STIC Search Report
EIC 1700

USPTO Scientific & Technical Information Center

STIC Database Tracking Number: 205202

TO: Gennadiy Mesh
Location: Rem 10D68
Art Unit : 1711
October 24, 2006

Case Serial Number: 10/787146

From: Kathleen Fuller
Location: EIC 1700
REMSEN 4B28
Phone: 571/272-2505
Kathleen.Fuller@uspto.gov

Search Notes

When I checked the structure/RN's for the applicant in Chemical Abstracts the structures did not match the structures in the claims. The applicant CA structures were more like starting porphyrin structures. I searched for porphyrin structures and combined the structures with utility and limited to dates of 2004 or earlier. This strategy would pick up the claim structures if they exist and are indexed as well as the simpler structures . I also did a subset search for 2 or more porphyrin structures with a metal and got 7,986 structures. This second set also was combined with utility and limited by date.

Please come and see me if you have questions.

STIC Search Results Feedback Form

USPTO

EIC17000

Questions about the scope or the results of the search? Contact *the EIC searcher or contact*:

Kathleen Fuller, EIC 1700 Team Leader
571/272-2505 REMSEN 4B28

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* ☐ *Example: 1713*
- *Relevant prior art found, search results used as follows:*

  ☐ 102 rejection

  ☐ 103 rejection

  ☐ Cited as being of interest.

  ☐ Helped examiner better understand the invention.

  ☐ Helped examiner better understand the state of the art in their technology.

  Types of relevant prior art found:

  ☐ Foreign Patent(s)

  ☐ Non-Patent Literature
  (journal articles, conference proceedings, new product announcements etc.)

- *Relevant prior art not found:*

  ☐ Results verified the lack of relevant prior art (helped determine patentability).

  ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

'OR OFFICIAL USE ONLY

ACCESS DB # 205202

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Scientific and Technical Information Center

SEARCH REQUEST FORM

equester's Full Name: Gennadij Mesh Examiner #: 82345 Date: Oct 19, 06
rt Unit: 1711 Phone Number: 2-2901 Serial Number: 10/787146
ocation (Bldg/Room#): Rem 10D88 Mailbox #): ________ Results Format Preferred (circle): PAPER DISK

****

) ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

itle of Invention: Element having pt phyrin ..

.ventors (please provide full names): Kobuke

arliest Priority Date: 02/28/2003

arch Topic:
ease provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the :cted species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. :fine any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

or Sequence Searches Only* *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the propriate serial number.*

) Formula (VIII) and (VIII')
in claim 1

2) Formulas in claim 3

) Formulas in claim 4

) Formula in claim 11

Please call before search !!

****

TAFF USE ONLY

rcher: K. Fuller	____ NA Sequence (#)	✓ STN ____ Dialog
rcher Phone #: ________	____ AA Sequence (#)	____ Questel/Orbit ____ Lexis/Nexis
ircher Location: ________	6 Structure (#)	____ Westlaw ____ WWW/Internet
e Searcher Picked Up: ________	____ Bibliographic	____ In-house sequence systems
te Completed: 10/24/06	____ Litigation	____ Commercial ____ Oligomer ____ Score/Length ____ Interference ____ SPDI ____ Encode/Transl
ircher Prep & Review Time: 40	____ Fulltext	________ Other (specify)
line Time: 60	____ Other	

subset search

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=> FILE REG
FILE 'REGISTRY' ENTERED AT 15:07:15 ON 24 OCT 2006
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DICTIONARY FILE UPDATES:   23 OCT 2006   HIGHEST RN 911100-17-9

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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FILE COVERS 1907 - 24 Oct 2006  VOL 145 ISS 18
FILE LAST UPDATED: 23 Oct 2006  (20061023/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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L3                STR
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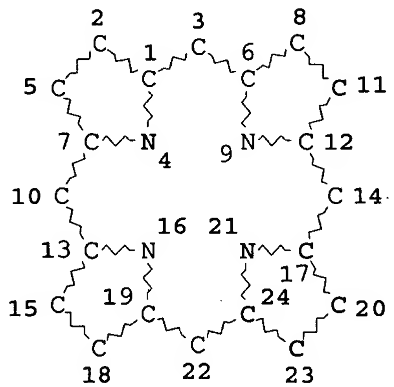

97,342 structures from this query

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

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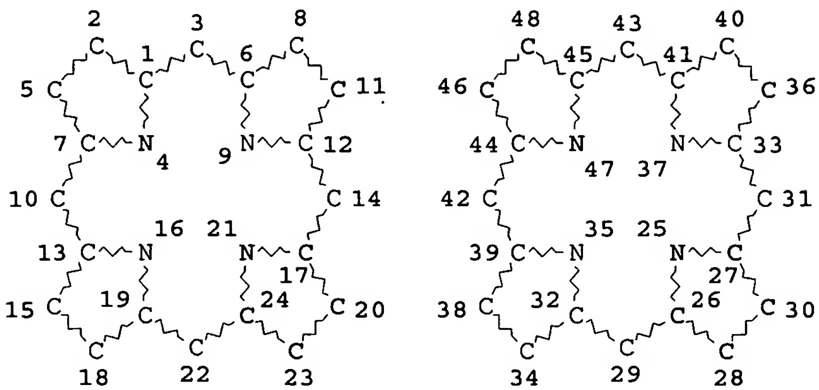
L10	82336	SEA FILE=HCAPLUS ABB=ON	L5
L12	465	SEA FILE=HCAPLUS ABB=ON	L10(L)SUBSTRATE?
L13	1	SEA FILE=HCAPLUS ABB=ON	L10(L)SUBSTRATE?(L)ANCHOR?
L14	5	SEA FILE=HCAPLUS ABB=ON	L10(L)SUBSTRATE?(L)COVALENT?
L15	1	SEA FILE=HCAPLUS ABB=ON	L12 AND PHOTOFUNC?
L16	5	SEA FILE=HCAPLUS ABB=ON	L12 AND MOLECULAR?(3A)DEVICE?
L17	3	SEA FILE=HCAPLUS ABB=ON	L12 AND (PHOTO? OR LIGHT?)(4A)?FUNC?
L18	36	SEA FILE=HCAPLUS ABB=ON	L12 AND OPTICAL?/SC,SX
L19	9	SEA FILE=HCAPLUS ABB=ON	L18 AND (DEV/RL OR DEVICE?)
L20	31	SEA FILE=HCAPLUS ABB=ON	L12(L)PREP/RL
L21	2	SEA FILE=HCAPLUS ABB=ON	L18 AND L20
L22	280	SEA FILE=HCAPLUS ABB=ON	L10 AND SUBSTRATE? AND OPTICAL?/SC,SX
L23	12667	SEA FILE=HCAPLUS ABB=ON	L10(L)PREP/RL
L24	44	SEA FILE=HCAPLUS ABB=ON	L22 AND L23
L25	12	SEA FILE=HCAPLUS ABB=ON	L24 AND (DEV/RL OR DEVICE?)
L26	29	SEA FILE=HCAPLUS ABB=ON	(L13 OR L14 OR L15 OR L16 OR L17) OR L19 OR L21 OR L25
L27		STR	



Subset search

10,312 structures from query

7,986 with metal

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

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L30     10312 SEA FILE=REGISTRY SUB=L5 SSS FUL L27
L31      7986 SEA FILE=REGISTRY ABB=ON  L30 AND M/ELS
L32      2733 SEA FILE=HCAPLUS ABB=ON  L31
L34        22 SEA FILE=HCAPLUS ABB=ON  L32 AND OPTICAL?/SC,SX AND SUBSTRATE?

L35        22 SEA FILE=HCAPLUS ABB=ON  L32 AND MOLECULAR?(3A)DEVICE?
L36        43 SEA FILE=HCAPLUS ABB=ON  L34 OR L35
L37        71 SEA FILE=HCAPLUS ABB=ON  L26 OR L36
L38         4 SEA FILE=HCAPLUS ABB=ON  L37 AND POLYMER?(4A)(SUBSTRATE? OR
              SURFACE?)
L40         6 SEA FILE=HCAPLUS ABB=ON  L37 AND POLYMER?(4A)?PORPHYRIN?
L41         7 SEA FILE=HCAPLUS ABB=ON  L37 AND POLYMER?/SC,SX
L42        12 SEA FILE=HCAPLUS ABB=ON  L37 AND POLYMER?
L43        14 SEA FILE=HCAPLUS ABB=ON  L38 OR L40 OR L41 OR L42
L44        71 SEA FILE=HCAPLUS ABB=ON  L37 OR L43
L45        57 SEA FILE=HCAPLUS ABB=ON  L44 AND (1840-2004)/PRY,AY,PY
L46         1 SEA FILE=HCAPLUS ABB=ON  L1 AND L45
```

=> D L46 IBIB ABS IND HITSTR

applicant note that the structures are different from those in the claims

L46 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:779367 HCAPLUS
DOCUMENT NUMBER: 141:304026
TITLE: **Substrate**-anchored covalent-bonded **porphyrin polymer functioning** as **photofunctional molecular device**
INVENTOR(S): Kobuke, Yoshiaki; Satake, Akiharu
PATENT ASSIGNEE(S): Nara Institute of Science and Technology, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 76 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
JP 2004266100	A2	20040924	JP 2003-54719		20030228	<--
US 2004202876	A1	20041014	US 2004-787146		20040227	<--
PRIORITY APPLN. INFO.:			JP 2003-54719	A	20030228	<--

OTHER SOURCE(S): MARPAT 141:304026

AB The invention relates to a covalent bonded **porphyrin polymer** anchored on a **substrate** by a linker mol., suited for use in making **photofunctional mol. devices**, such as an organic solar cell and a 3rd order nonlinear optical **device.**

IC ICM H01L051-00
ICS G02F001-361; H01L031-04; H01M014-00; C07D487-22

CC 73-11 (**Optical**, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): **35**, 52, 74, 78

ST **porphyrin polymer** covalent bond anchored **photofunctional mol device**

IT Nonlinear optical materials
Optical materials
(**substrate**-anchored covalent-bonded **porphyrin polymer functioning** as **photofunctional mol. device**)

IT Porphyrins
RL: **DEV (Device component use)**; USES (Uses)
(**substrate**-anchored covalent-bonded **porphyrin polymer functioning** as **photofunctional mol. device**)

IT **763139-61-3DP**, reaction with zinc porphyrin functionalized gold and oligomeric dizincporphyrin **763139-63-5DP**, gold **surface** supported, **polymerization** with **biszincporphyrin**, reaction product with pyrrazolofullerene zinc porphyrin **763139-64-6DP**, reaction with zinc porphyrin functionalized gold, terminated with pyrrazolofullerene zinc porphyrin
RL: **DEV (Device component use)**; SPN (Synthetic preparation); **PREP (Preparation)**; USES (Uses)
(**substrate-anchored covalent**-bonded **porphyrin polymer functioning** as **photofunctional mol. device**)

IT 79-37-8, Ethanedioyl dichloride 98-59-9, p-Toluenesulfonyl chloride 106-95-6, Allylbromide, reactions 107-18-6, Allylalcohol, reactions 107-97-1, n-Methylglycine 109-97-7, Pyrrol 557-34-6, Zinc acetate 623-27-8, Terephthalaldehyde 7647-01-0, Hydrochloric acid, reactions 10387-40-3, Potassium thioacetate 13750-81-7, 2-Formyl-1-methylimidazole 13865-19-5, Methoxycarbonylpropanal 25265-75-2, Butanediol 26153-38-8, 3,5-Dihydroxybenzaldehyde 30525-89-4, Paraformaldehyde 53463-68-6 99685-96-8, Fullerene c60
RL: RCT (Reactant); RACT (Reactant or reagent)
(**substrate**-anchored covalent-bonded **porphyrin polymer functioning** as **photofunctional mol. device**)

IT 1471-15-4P, 4-Allyloxy-1-butanol 63880-78-4P 646502-39-8P 676593-76-3P 763108-86-7P 763108-87-8P 763108-88-9P **763108-89-0P 763108-90-3P 763108-91-4P 763108-92-5P 763108-93-6P 763108-94-7P 763108-95-8P 763139-60-2P 763139-61-3P 763139-62-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**substrate-anchored covalent**-bonded **porphyrin polymer functioning** as **photofunctional mol. device)**

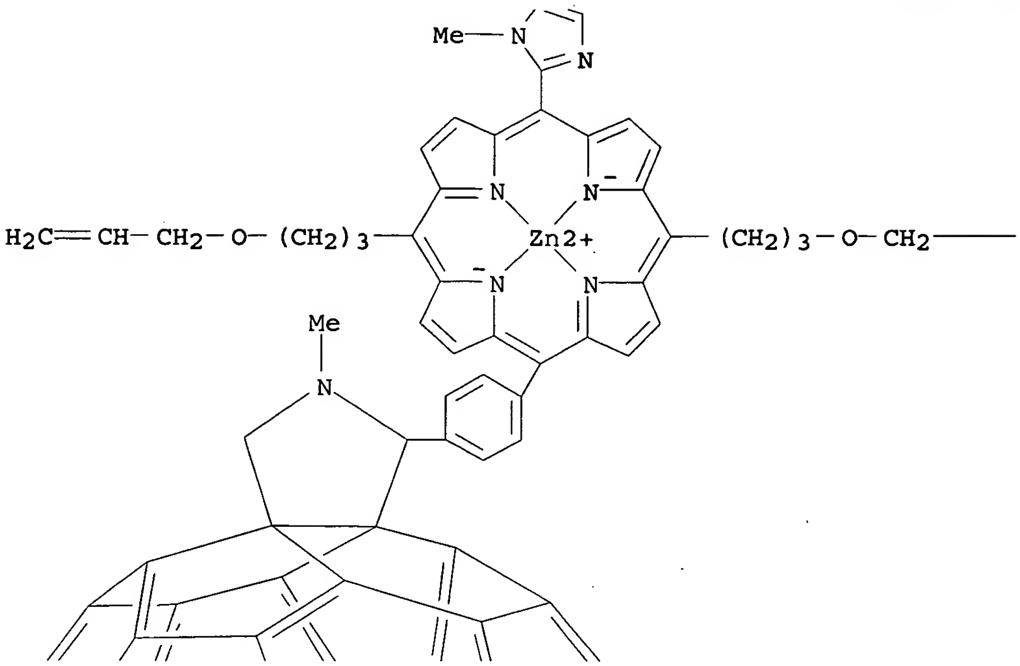
IT **763139-61-3DP**, reaction with zinc porphyrin functionalized gold and oligomeric dizincporphyrin **763139-63-5DP**, gold **surface** supported, **polymerization** with **biszincporphyrin** , reaction product with pyrrazolofullerene zinc porphyrin **763139-64-6DP**, reaction with zinc porphyrin functionalized gold, terminated with pyrrazolofullerene zinc porphyrin
RL: **DEV (Device component use)**; SPN (Synthetic preparation); **PREP (Preparation)**; USES (Uses)
(**substrate-anchored covalent**-bonded **porphyrin polymer functioning** as **photofunctional mol. device)**

RN 763139-61-3 HCAPLUS

CN Zinc, [1',5'-dihydro-1'-methyl-2'-[4-[15-(1-methyl-1H-imidazol-2-yl)-10,20-bis[3-(2-propenyloxy)propyl]-21H,23H-porphin-5-yl-κN21,κN22,κN23,κN24]phenyl]-2'H-[5,6]fullereno-C60-Ih-[1,9-c]pyrrolato(2-)]-, (SP-4-2)-, (9CI) (CA INDEX NAME)

PAGE 1-A

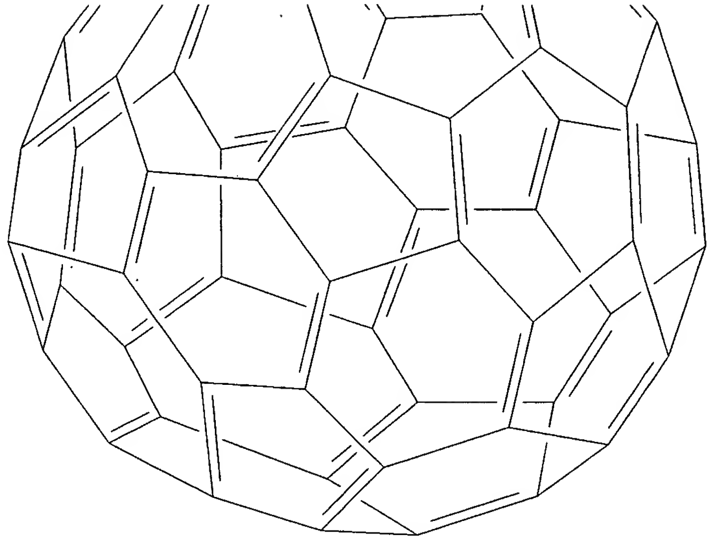
PAGE 2-A



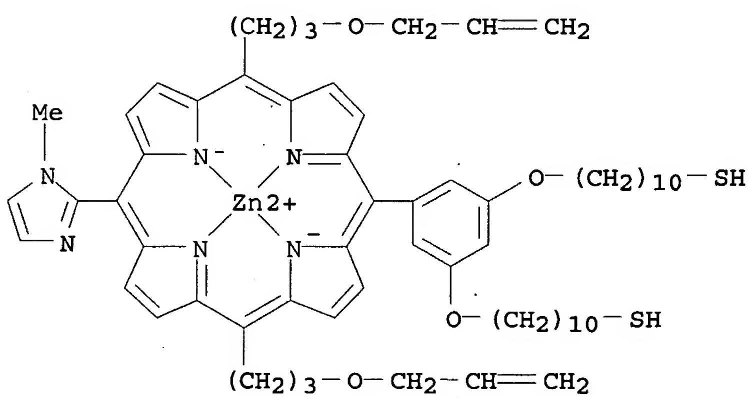
PAGE 2-B

— CH═CH2

PAGE 3-A



RN 763139-63-5 HCAPLUS
CN Zinc, [[10,10'-[[5-[15-(1-methyl-1H-imidazol-2-yl)-10,20-bis[3-(2-propenyloxy)propyl]-21H,23H-porphin-5-yl-κN21,κN22,κN23,κN24]-1,3-phenylene]bis(oxy)]bis[1-decanethiolato]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

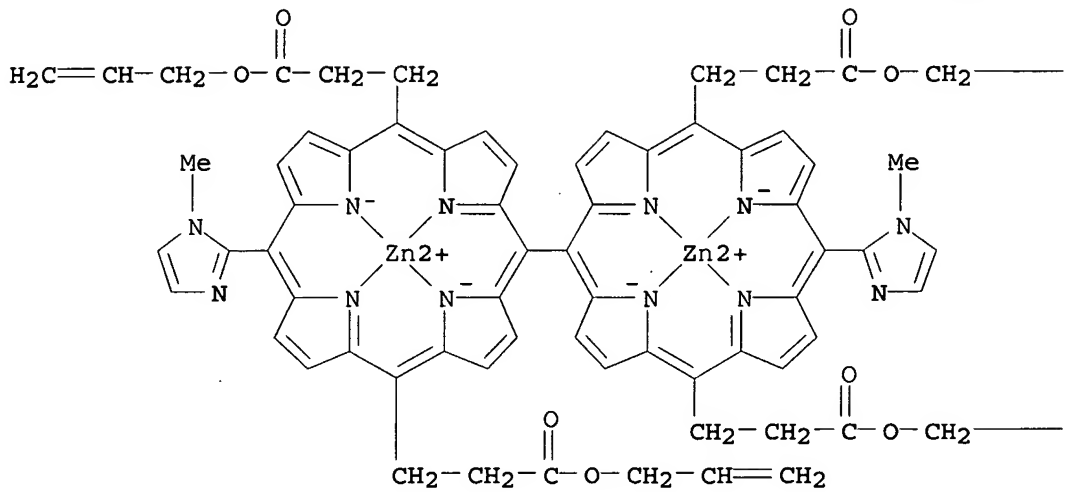


RN 763139-64-6 HCAPLUS
CN Zinc, [μ-[tetra-2-propenyl 15,15'-bis(1-methyl-1H-imidazol-2-yl)[5,5'-bi-21H,23H-porphine]-10,10',20,20'-tetrapropanoato(4-)-κN21,κN22,κN23,κN24:κN21',κN22',.kappa.N23',κN24']]di-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 763139-62-4
CMF C72 H62 N12 O8 Zn2
CCI CCS

PAGE 1-A



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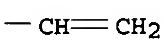
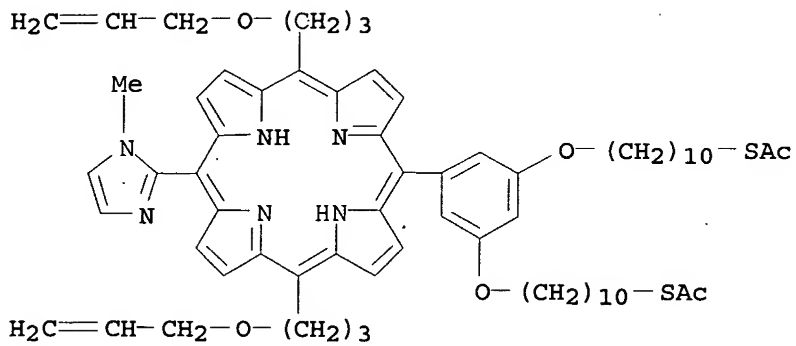


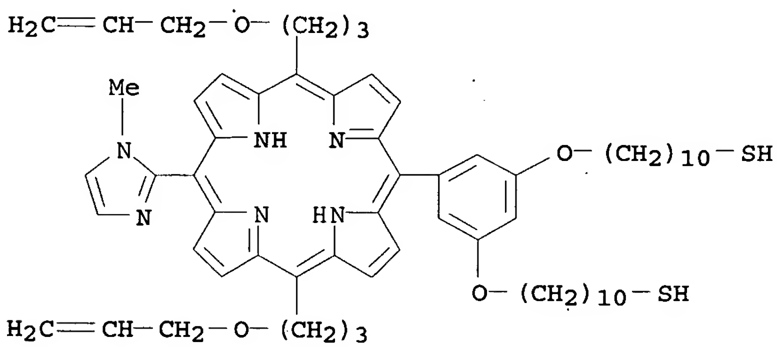
IT **763108-89-0P 763108-90-3P 763108-91-4P**
763108-92-5P 763108-93-6P 763108-94-7P
763108-95-8P 763139-60-2P 763139-61-3P
763139-62-4P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**
(Preparation); RACT (Reactant or reagent)
(**substrate-anchored covalent**-bonded
porphyrin polymer functioning as
photofunctional mol. device)

RN 763108-89-0 HCAPLUS

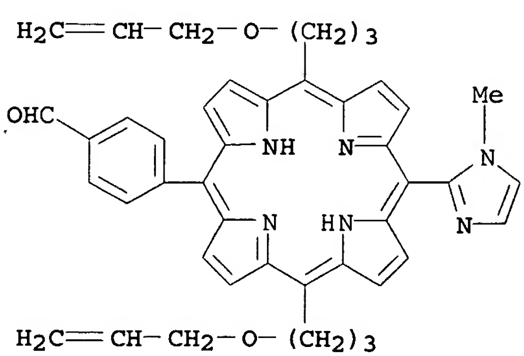
CN Ethanethioic acid, S,S'-[[5-[15-(1-methyl-1H-imidazol-2-yl)-10,20-bis[3-(2-propenyloxy)propyl]-21H,23H-porphin-5-yl]-1,3-phenylene]bis(oxy-10,1-decanediyl)] ester (9CI) (CA INDEX NAME)



RN 763108-90-3 HCAPLUS
CN 1-Decanethiol, 10,10'-[[5-[15-(1-methyl-1H-imidazol-2-yl)-10,20-bis[3-(2-propenyloxy)propyl]-21H,23H-porphin-5-yl]-1,3-phenylene]bis(oxy)]bis- (9CI) (CA INDEX NAME)

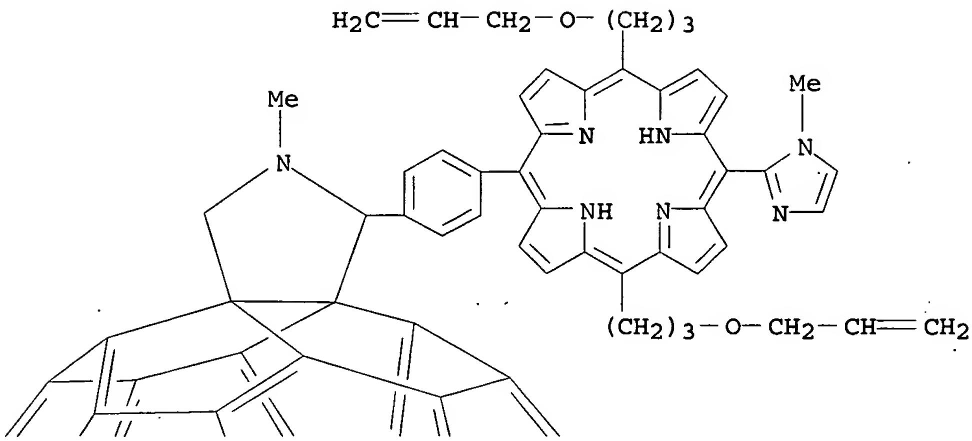


RN 763108-91-4 HCAPLUS
CN Benzaldehyde, 4-[15-(1-methyl-1H-imidazol-2-yl)-10,20-bis[3-(2-propenyloxy)propyl]-21H,23H-porphin-5-yl]- (9CI) (CA INDEX NAME)



RN 763108-92-5 HCAPLUS
CN 2'H-[5,6]Fullereno-C60-Ih-[1,9-c]pyrrole, 1',5'-dihydro-1'-methyl-2'-[4-[15-(1-methyl-1H-imidazol-2-yl)-10,20-bis[3-(2-propenyloxy)propyl]-21H,23H-porphin-5-yl]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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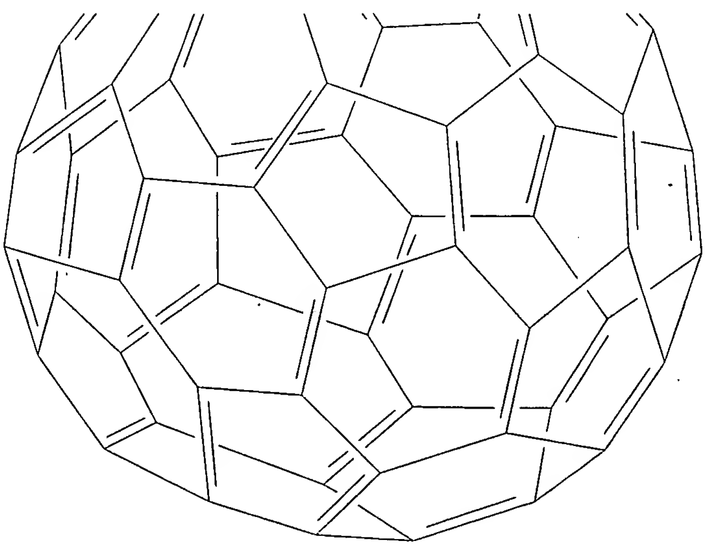
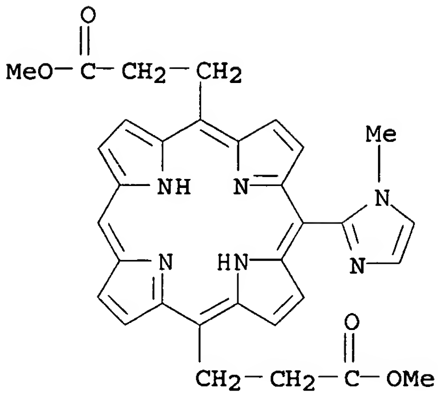
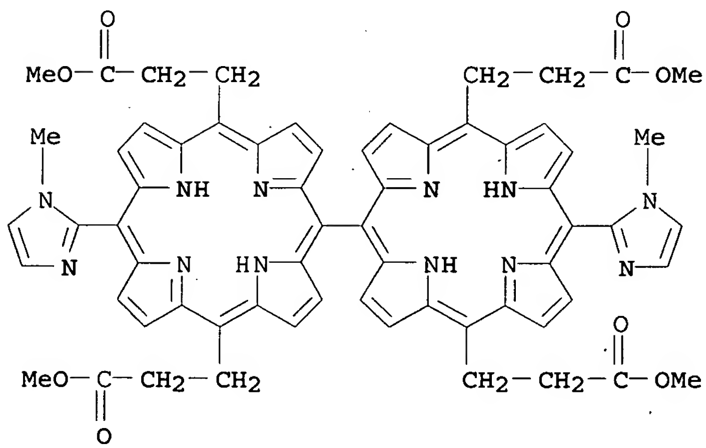


RN 763108-93-6 HCAPLUS
CN 21H,23H-Porphine-5,15-dipropanoic acid, 10-(1-methyl-1H-imidazol-2-yl)-, dimethyl ester (9CI) (CA INDEX NAME)

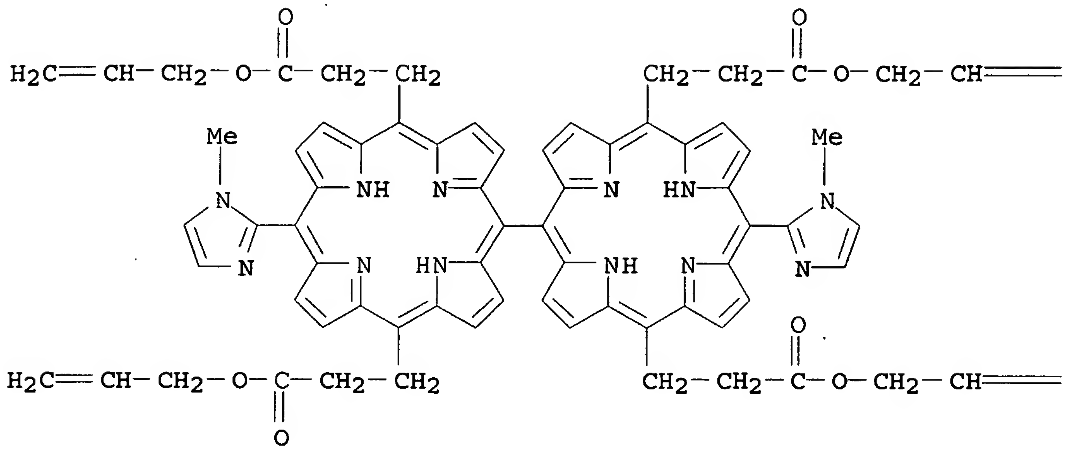


RN 763108-94-7 HCAPLUS
CN [5,5'-Bi-21H,23H-porphine]-10,10',20,20'-tetrapropanoic acid, 15,15'-bis(1-methyl-1H-imidazol-2-yl)-, tetramethyl ester (9CI) (CA INDEX NAME)



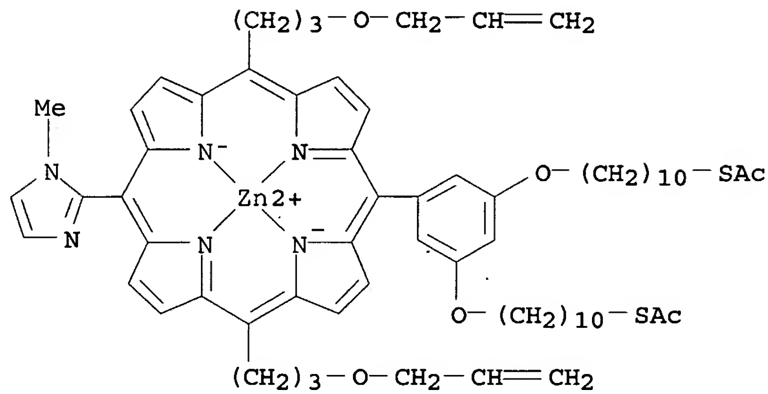
RN 763108-95-8 HCAPLUS
CN [5,5'-Bi-21H,23H-porphine]-10,10',20,20'-tetrapropanoic acid, 15,15'-bis(1-methyl-1H-imidazol-2-yl)-, tetra-2-propenyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

RN 763139-60-2 HCAPLUS
CN Zinc, [[S,S'-[[5-[15-(1-methyl-1H-imidazol-2-yl)-10,20-bis[3-(2-propenyloxy)propyl]-21H,23H-porphin-5-yl-κN21,κN22,κN23,κN24]-1,3-phenylene]bis(oxy-10,1-decanediyl)] diethanethioato](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



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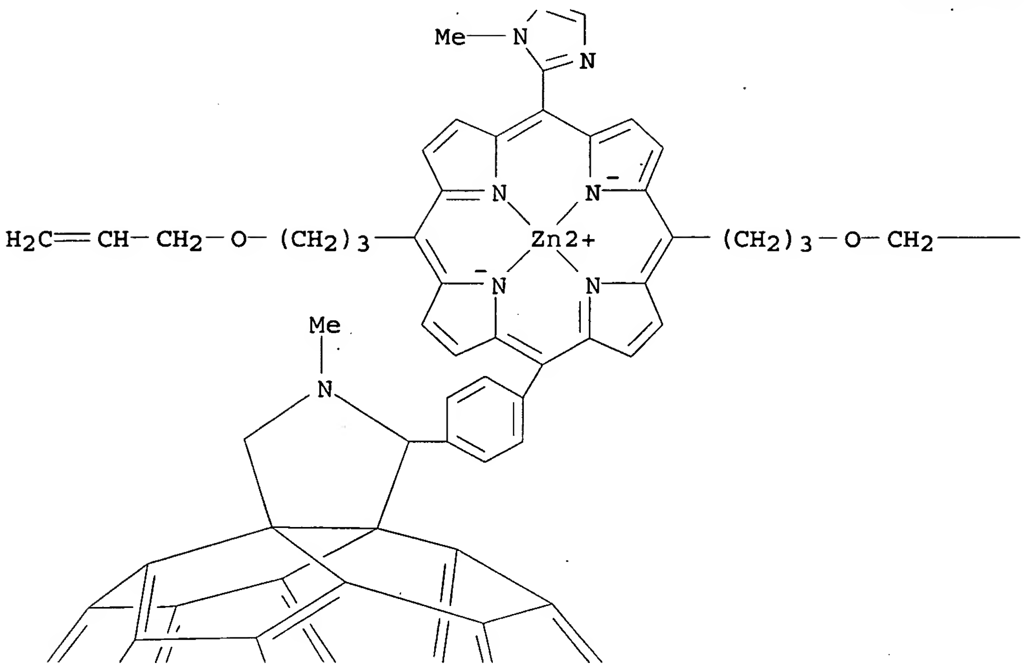
CN Zinc, [1',5'-dihydro-1'-methyl-2'-[4-[15-(1-methyl-1H-imidazol-2-yl)-10,20-bis[3-(2-propenyloxy)propyl]-21H,23H-porphin-5-yl-κN21,κN22,κN23,κN24]phenyl]-2'H-[5,6]fullereno-C60-Ih-[1,9-c]pyrrolato(2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A



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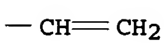

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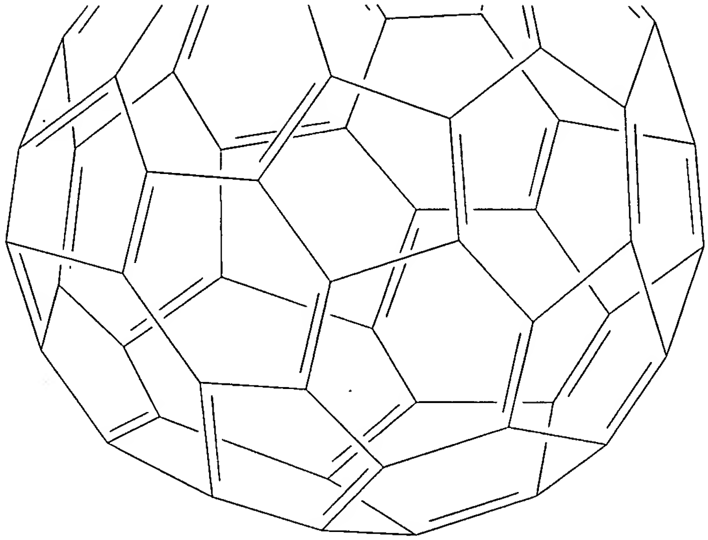
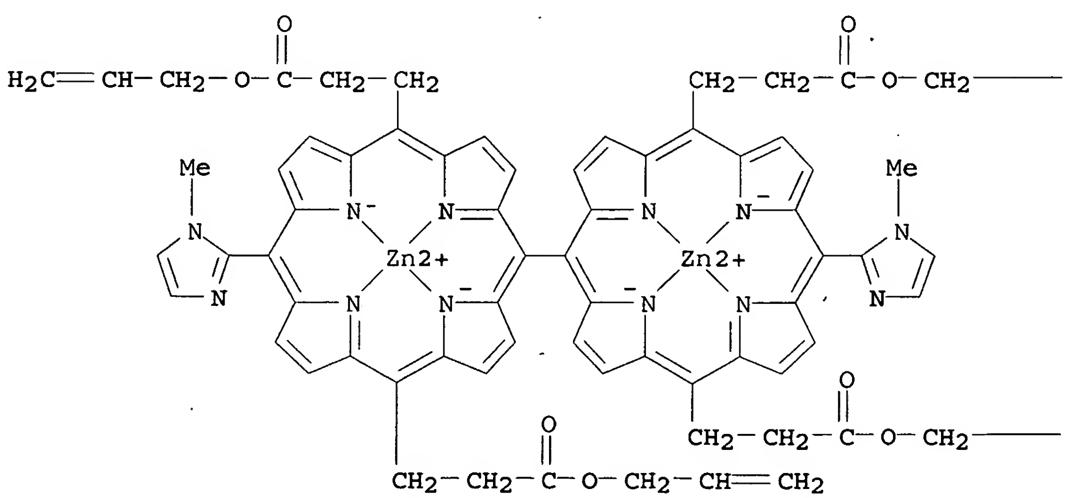


RN 763139-62-4 HCAPLUS
CN Zinc, [μ-[tetra-2-propenyl 15,15'-bis(1-methyl-1H-imidazol-2-yl)[5,5'-bi-21H,23H-porphine]-10,10',20,20'-tetrapropanoato(4-)-κN21,κN22,κN23,κN24:κN21',κN22',.kappa .N23',κN24']]di- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— $CH=CH_2$

— $CH=CH_2$

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=>  S L45 NOT L46
L47          56 L45 NOT L46

=>  D QUE L47
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L3                STR
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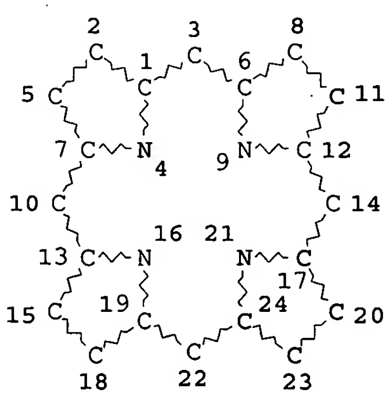

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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  24

STEREO ATTRIBUTES: NONE
L5          97342 SEA FILE=REGISTRY SSS FUL L3
L10         82336 SEA FILE=HCAPLUS ABB=ON  L5
L12           465 SEA FILE=HCAPLUS ABB=ON  L10(L)SUBSTRATE?
L13             1 SEA FILE=HCAPLUS ABB=ON  L10(L)SUBSTRATE?(L)ANCHOR?
L14             5 SEA FILE=HCAPLUS ABB=ON  L10(L)SUBSTRATE?(L)COVALENT?
L15             1 SEA FILE=HCAPLUS ABB=ON  L12 AND PHOTOFUNC?
L16             5 SEA FILE=HCAPLUS ABB=ON  L12 AND MOLECULAR?(3A)DEVICE?
```

```
L17             3 SEA FILE=HCAPLUS ABB=ON  L12 AND (PHOTO? OR LIGHT?)(4A)?FUNC?
L18            36 SEA FILE=HCAPLUS ABB=ON  L12 AND OPTICAL?/SC,SX
L19             9 SEA FILE=HCAPLUS ABB=ON  L18 AND (DEV/RL OR DEVICE?)
L20            31 SEA FILE=HCAPLUS ABB=ON  L12(L)PREP/RL
L21             2 SEA FILE=HCAPLUS ABB=ON  L18 AND L20
L22           280 SEA FILE=HCAPLUS ABB=ON  L10 AND SUBSTRATE? AND OPTICAL?/SC,SX

L23         12667 SEA FILE=HCAPLUS ABB=ON  L10(L)PREP/RL
L24            44 SEA FILE=HCAPLUS ABB=ON  L22 AND L23
L25            12 SEA FILE=HCAPLUS ABB=ON  L24 AND (DEV/RL OR DEVICE?)
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                L19 OR L21 OR L25
L27             STR
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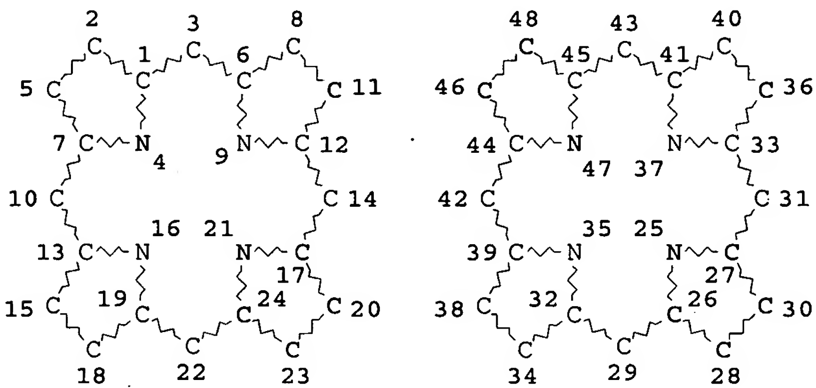

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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  48

STEREO ATTRIBUTES: NONE
L30         10312 SEA FILE=REGISTRY SUB=L5 SSS FUL L27
L31          7986 SEA FILE=REGISTRY ABB=ON  L30 AND M/ELS
L32          2733 SEA FILE=HCAPLUS ABB=ON  L31
L34            22 SEA FILE=HCAPLUS ABB=ON  L32 AND OPTICAL?/SC,SX AND SUBSTRATE?

L35            22 SEA FILE=HCAPLUS ABB=ON  L32 AND MOLECULAR?(3A)DEVICE?
L36            43 SEA FILE=HCAPLUS ABB=ON  L34 OR L35
L37            71 SEA FILE=HCAPLUS ABB=ON  L26 OR L36
L38             4 SEA FILE=HCAPLUS ABB=ON  L37 AND POLYMER?(4A)(SUBSTRATE? OR
                SURFACE?)
L40             6 SEA FILE=HCAPLUS ABB=ON  L37 AND POLYMER?(4A)?PORPHYRIN?
L41             7 SEA FILE=HCAPLUS ABB=ON  L37 AND POLYMER?/SC,SX
L42            12 SEA FILE=HCAPLUS ABB=ON  L37 AND POLYMER?
L43            14 SEA FILE=HCAPLUS ABB=ON  L38 OR L40 OR L41 OR L42
L44            71 SEA FILE=HCAPLUS ABB=ON  L37 OR L43
L45            57 SEA FILE=HCAPLUS ABB=ON  L44 AND (1840-2004)/PRY,AY,PY
L46             1 SEA FILE=HCAPLUS ABB=ON  L1 AND L45
L47            56 SEA FILE=HCAPLUS ABB=ON  L45 NOT L46
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Remaining 56 CA references

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=> SEL HIT RN L47 1-56
E1 THROUGH E310 ASSIGNED
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310 structures/RN's in the 56 references so one structure only printed for each references

=> D L47 1-56 IBIB ABS IND FHITSTR

L47 ANSWER 1 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:182320 HCAPLUS
DOCUMENT NUMBER: 142:289339
TITLE: High temperature attachment of organic molecules to substrates
INVENTOR(S): Bocian, David F.; Lindsey, Jonathan; Liu, Zhiming; Yasseri, Amir A.; Misra, Veen; Zhao, Qian; Li, Qiliang; Surthi, Shyam; Loewe, Robert S.
PATENT ASSIGNEE(S): The Regents of the University of California, USA
SOURCE: U.S. Pat. Appl. Publ., 35 pp., Cont.-in-part of U.S. Ser. No. 628,868.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005048691	A1	20050303	US 2003-742596	20031219 <--
US 2005019500	A1	20050127	US 2003-628868	20030728 <--
US 6943054	B2	20050913		
WO 2005043583	A2	20050512	WO 2004-US24105	20040726 <--
WO 2005043583	A3	20051208		

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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1649526	A2	20060426	EP 2004-816786	20040726 <--

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PRIORITY APPLN. INFO.:

APPLICATION NO.		DATE
US 2003-489992P	P	20030725 <--
US 2003-628868	A2	20030728 <--
US 2003-742596	A	20031219 <--
WO 2004-US24105	W	20040726 <--

AB This invention provides a new procedure for attaching mols. to semiconductor surfaces, in particular Si. The mols., which include, but are not limited to porphyrins and ferrocenes, were previously shown to be attractive candidates for mol.-based information storage. The new attachment procedure is simple, can be completed in short times, requires minimal amts. of material, is compatible with diverse mol. functional groups, and in some instances affords unprecedented attachment motifs. These features greatly enhance the integration of the mol. materials into the processing steps that are needed to create hybrid **mol ./semiconductor** information storage **devices.**

IC ICM H01L051-40
ICS H01L021-26; H01L021-477

INCL 438099000; 438795000

CC 76-3 (Electric Phenomena)
Section cross-reference(s): 48, 66

ST org mol attachment semiconductor substrate information storage
IT Vapor deposition process
(chemical; high temperature attachment of organic mols. to substrates for information storage systems)
IT Porphyrins
RL: CPS (Chemical process); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(complexes; high temperature attachment of organic mols. to substrates for information storage systems)
IT Coating materials
Coating process
Diodes
Etching
Functional groups
Gate contacts
Heat treatment
Hybrid organic-inorganic materials
Integrated circuits
Lithography
Molecular beam epitaxy
Molecules
Rectifiers
Redox reaction
Semiconductor device fabrication
Semiconductor devices
Semiconductor materials
Semiconductor materials
Semiconductor memory devices
Sputtering
Transistors
(high temperature attachment of organic mols. to substrates for information storage systems)
IT Porphyrins
RL: CPS (Chemical process); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(high temperature attachment of organic mols. to substrates for information storage systems)
IT Alkaline earth oxides
Group IVA elements
Transition metal nitrides
Transition metal oxides
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PYP (Physical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
(high temperature attachment of organic mols. to substrates for information storage systems)
IT Alkaline earth pnictides
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PYP (Physical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
(nitrides; high temperature attachment of organic mols. to substrates for information storage systems)
IT Vapor deposition process
(plasma; high temperature attachment of organic mols. to substrates for information storage systems)
IT **Porphyrins**
RL: CPS (Chemical process); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(**polymers**; high temperature attachment of organic mols. to substrates for information storage systems)

IT Coating process
(spray; high temperature attachment of organic mols. to substrates for information storage systems)
IT Information systems
(storage; high temperature attachment of organic mols. to substrates for information storage systems)
IT **827322-27-0 827322-28-1**
RL: CPS (Chemical process); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(Type c triple decker; high temperature attachment of organic mols. to **substrates** for information storage systems)
IT 1333-74-0, Hydrogen, processes **150152-74-2 150676-43-0**
184153-94-4 210905-79-6 211999-48-3
211999-54-1 211999-56-3 247069-46-1
247103-29-3 307538-15-4 468095-54-7
485370-19-2 501011-89-8 502613-00-5
651033-96-4 651033-97-5 651034-10-5
753459-98-2 753459-99-3 753460-04-7
753460-05-8 753460-21-8 784151-82-2
820233-67-8 827314-46-5 827314-57-8
827314-59-0 827314-64-7 827314-73-8
827314-75-0 827314-77-2 827314-79-4
827314-85-2 827314-87-4 827314-89-6
RL: CPS (Chemical process); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(high temperature attachment of organic mols. to **substrates** for information storage systems)
IT 1313-96-8, Niobium oxide (Nb2O5) 1314-35-8, Tungsten trioxide, processes
1314-61-0, Tantalum oxide (Ta2O5) 7440-03-1, Niobium, processes
7440-21-3, Silicon, processes 7440-25-7, Tantalum, processes
7440-33-7, Tungsten, processes 7440-56-4, Germanium, processes
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PYP (Physical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
(high temperature attachment of organic mols. to substrates for information storage systems)
IT **827322-27-0**
RL: CPS (Chemical process); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(Type c triple decker; high temperature attachment of organic mols. to **substrates** for information storage systems)
RN 827322-27-0 HCAPLUS
CN Europium, [5,15-bis[4-(1,1-dimethylethyl)phenyl]-10,20-bis(4-ethynylphenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,.ka
ppa.N24][μ-[C,C,C,C-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,κN32:κN2
9,κN30,κN31,κN32]][C,C,C,C-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,κN32]d
i- (9CI) (CA INDEX NAME)

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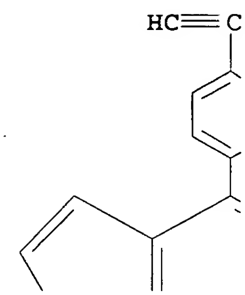

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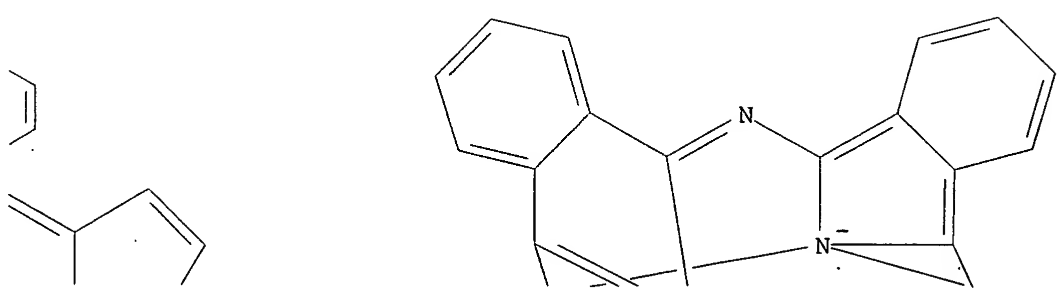

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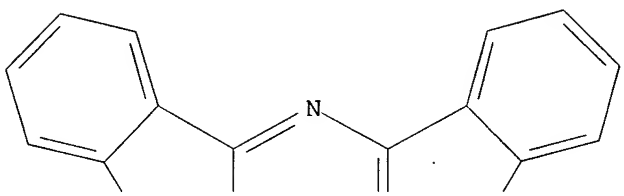

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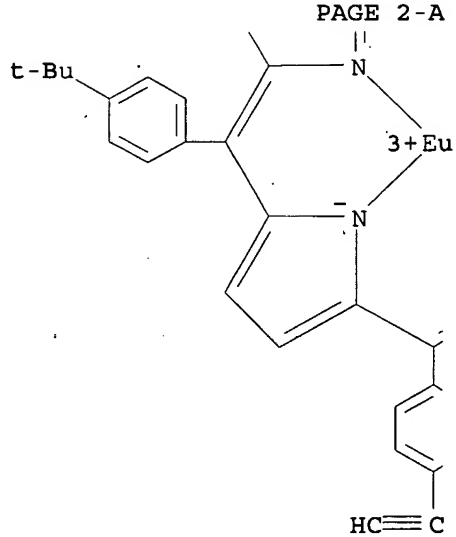

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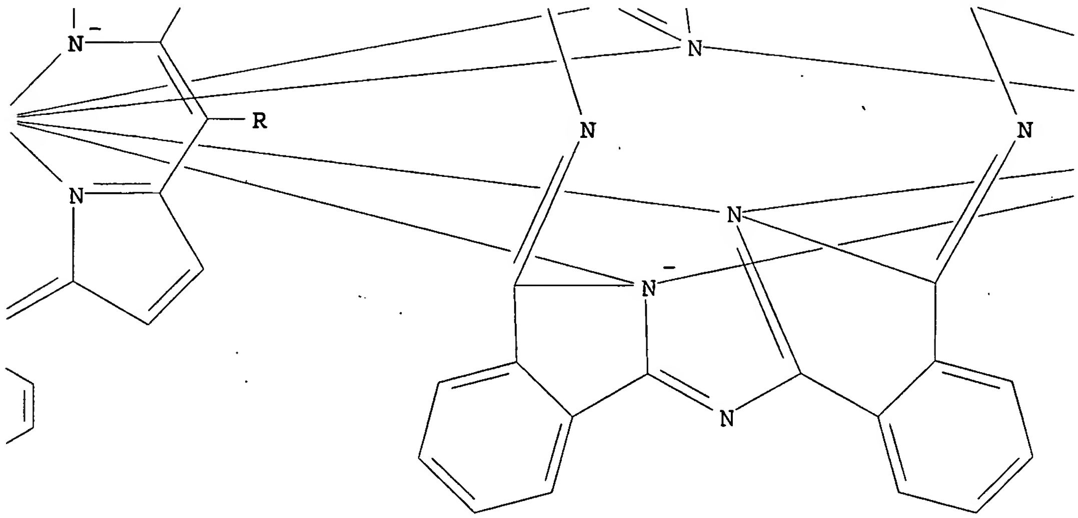

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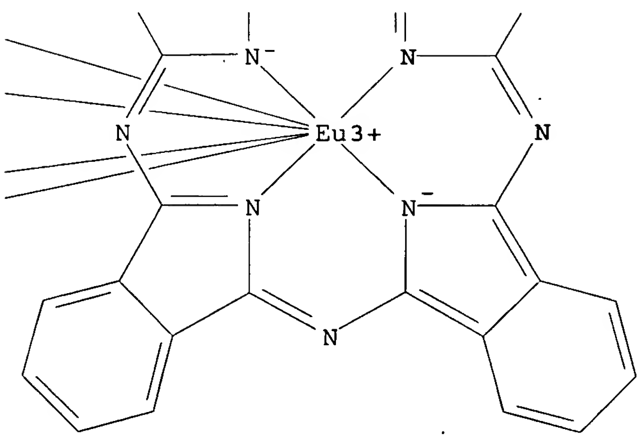
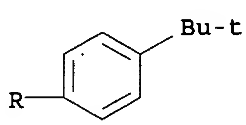


PAGE 3-A



8 (D1—Bu-t)

L47 ANSWER 2 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:77999 HCAPLUS
DOCUMENT NUMBER: 142:167539

TITLE: Covalently attachment of organic molecules to group III, IV or V substrates as information storage device
INVENTOR(S): Bocian, David F.; Lindsey, Jonathan S.; Liu, Zhiming; Yasseri, Amir A.; Loewe, Robert S.
PATENT ASSIGNEE(S): The Regents of the University of California, USA
SOURCE: U.S. Pat. Appl. Publ., 22 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005019500	A1	20050127	US 2003-628868	20030728 <--
US 6943054	B2	20050913		
US 2005048691	A1	20050303	US 2003-742596	20031219 <--
WO 2005043583	A2	20050512	WO 2004-US24105	20040726 <--
WO 2005043583	A3	20051208		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1649526	A2	20060426	EP 2004-816786	20040726 <--

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005217559	A1	20051006	US 2005-140011	20050526 <--

PRIORITY APPLN. INFO.:
US 2003-489992P P 20030725 <--
US 2003-628868 A2 20030728 <--
US 2003-742596 A 20031219 <--
WO 2004-US24105 W 20040726 <--

AB A procedure for attaching mols. to semiconductor surfaces, in particular silicon, is simple, can be completed in short times, requires minimal amts. of material, is compatible with diverse mol. functional groups, and in some instances affords unprecedented attachment motifs. The mols., which include, but are not limited to porphyrins and ferrocenes, have been previously shown to be attractive candidates for mol.-based information storage. These features greatly enhance the integration of the mol. materials into the processing steps that are needed to create hybrid **mol.**/semiconductor information storage **devices.** Such a method of covalently coupling an organic mol. to a surface of a Group III, IV, or V element or to a semiconductor comprising a Group III, IV, or V element, comprises the steps of: providing a heat resistant organic mol. derivatized with an attachment group; and contacting the derivatized heat resistant organic mol. with a surface of said Group III, IV, or V element or semiconductor comprising a Group III, IV, or V element; and heating the surface to a temperature of at least about 200° C. whereby said attachment group forms a covalent bond with said surface.

IC ICM B05D003-02
ICS H01M004-60
INCL 427384000; 429213000
CC 76-3 (Electric Phenomena)
ST porphyrin silicon information storage medium

IT Diodes
Electrochemical cells
Integrated circuits
Memory devices
Rectifiers
Semiconductor device fabrication
Semiconductor materials
Transistors
(covalently attachment of organic mols. to group III, IV or V substrates as information storage device)

IT Porphyrins
RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
(covalently attachment of organic mols. to group III, IV or V substrates as information storage device)

IT Integrated circuits
(gates; covalently attachment of organic mols. to group III, IV or V substrates as information storage device)

IT **150152-74-2**, 5-(4-Ethynylphenyl)-10,15,20-trimesitylporphinatozinc(II) **150676-43-0**, 5-[4-[2-(Trimethylsilyl)ethynyl]phenyl]-10,15,20-tri-p-tolylporphinat ozinc(II) **184153-94-4**, 5-[4-[2-(Trimethylsilyl)ethynyl]phenyl]-10,15,20-trimesitylporphinato zinc(II) **210905-79-6**, 5,15-Bis(4-iodophenyl)-10,20-dimesitylporphinatozinc(II) **211999-48-3**, 5,10-Bis(4-ethynylphenyl)-15,20-dimesitylporphinatozinc(II) **211999-54-1**, 5,10-Bis(4-iodophenyl)-15,20-dimesitylporphinatozinc(II) **211999-56-3**, 5,10-Bis[4-[2-(trimethylsilyl)ethynyl]phenyl]-15,20-dimesitylporphina tozinc(II) **247069-46-1**, 5,15-Bis(4-ethynylphenyl)-10,20-dimesitylporphinatozinc(II) **247103-29-3**, 5-(4-Iodophenyl)-10,15,20-trimesitylporphinatozinc(II) **251989-85-2**, 5-[4-(S-Acetylthiomethyl)phenyl]-10,15,20-trimesitylporphinatozinc(II) **468095-54-7**, 5-(3,5-Diethynylphenyl)-10,15,20-trimesitylporphinatozinc(II) **485370-19-2**, 5-[4-(Hydroxymethyl)phenyl]-10,15,20-trimesitylporphinatozinc(II) **501011-89-8**, 5-(4-Bromophenyl)-10,15,20-tri-p-tolylporphinatozinc(II) **502613-00-5**, 5,10,15,20-Tetrakis(4-ethynylphenyl)porphinatozinc(II) **632301-78-1**, 5,15-Bis(4-ethynylphenyl)-10,20-bis(4-tert-butylphenyl)porphinatozinc(II) **632301-82-7**, 5,15-Bis(4-ethynylphenyl)porphinatozinc(II) **651033-96-4**, 5-(4-Bromomethylphenyl)-10,15,20-trimesitylporphinatozinc(II) **651033-97-5**, 5-[4-(Mercaptomethyl)phenyl]-10,15,20-trimesitylporphinatozinc(II) **651034-10-5**, 5-(4-Hydroxyphenyl)-10,15,20-trimesitylporphinatozinc(II) **753459-98-2**, 5-(4-Vinylphenyl)-10,15,20-trimesitylporphinatozinc(II) **753459-99-3**, 5-(4-Allylphenyl)-10,15,20-trimesitylporphinatozinc(II) **753460-04-7**, 5-(4-Vinylphenyl)-10,15,20-tri-p-tolylporphinatozinc(II) **753460-05-8**, 5-(4-Allylphenyl)-10,15,20-tri-p-tolylporphinatozinc(II) **753460-21-8** **784151-82-2**, 5-[4-(Hydroxymethyl)phenyl]-10,15,20-tri-p-tolylporphinatozinc(II) **820233-67-8**, 5-(Hydroxymethyl)-10,15,20-trimesitylporphinatozinc(II) **827314-46-5**, 5-(4-Formylphenyl)-15-phenyl-10,20-di-p-tolylporphinatozinc(II) **827314-57-8**, 5-[4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-10,20-bis(3,5-di-tert-butylphenyl)-15-mesitylporphinatozinc(II) **827314-59-0**, 5-Iodo-10,20-bis(3,5-di-tert-butylphenyl)-15-mesitylporphinatozinc(II) **827314-64-7**, 5,10,15-Tris(4-ethynylphenyl)-20-mesitylporphinatozinc(II) **827314-68-1**, 5,15-Bis(3-ethynylphenyl)-10,20-dimesitylporphinatozinc(II) **827314-73-8**

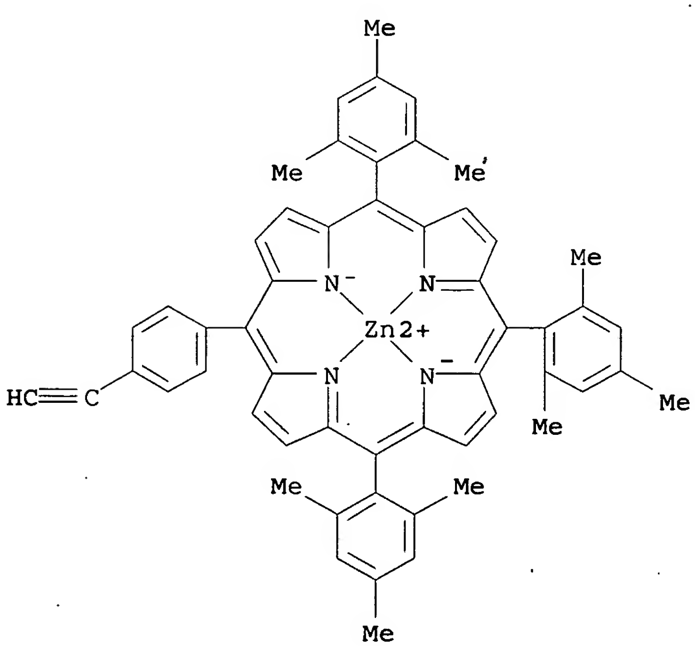
827314-75-0, 5-(4-Iodophenyl)-10,20-bis(3,5-di-tert-butylphenyl)-15-mesitylporphinatozinc(II) **827314-77-2**, 5,10-Bis(4-ethynylphenyl)-15,20-bis(4-tert-butylphenyl)porphinatozinc(II) **827314-79-4** **827314-85-2** **827314-87-4**, 5,10-Bis[4-[2-(triisopropylsilyl)ethynyl]biphen-4'-yl]-15,20-bis(4-tert-butylphenyl)porphinatozinc(II) **827314-89-6**, 5,10-Bis[4-[2-(triisopropylsilyl)ethynyl]phenyl]-15,20-bis(4-tert-butylphenyl)porphinatozinc(II) **827322-27-0** **827322-28-1**
RL: DEV (Device component use); RCT (Reactant); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)
(**covalently** attachment of organic mols. to group III, IV or V **substrates** as information storage device)

IT 102-54-5D, Ferrocene, derivative 7440-21-3D, Silicon, optionally doped 7440-56-4D, Germanium, optionally doped
RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
(covalently attachment of organic mols. to group III, IV or V substrates as information storage device)

IT **150152-74-2**, 5-(4-Ethynylphenyl)-10,15,20-trimesitylporphinatozinc(II)
RL: DEV (Device component use); RCT (Reactant); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)
(**covalently** attachment of organic mols. to group III, IV or V **substrates** as information storage device)

RN 150152-74-2 HCAPLUS

CN Zinc, [5-(4-ethynylphenyl)-10,15,20-tris(2,4,6-trimethylphenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-2)-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

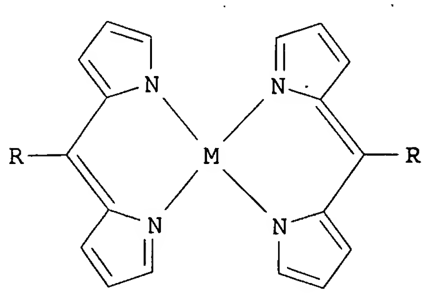
L47 ANSWER 3 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:1080724 HCAPLUS

DOCUMENT NUMBER: 142:48011
TITLE: Methods and intermediates for the synthesis of dipyrrin-substituted porphyrinic macrocycles for use in data storage devices and light harvesting arrays
INVENTOR(S): Yu, Lianhe; Muthukumaran, Kannan; Sreedharan, Prathapan; Lindsey, Jonathan S.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 27 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004254383	A1	20041216	US 2003-456321	20030606 <--
WO 2004109768	A2	20041216	WO 2004-US18477	20040603 <--
WO 2004109768	A3	20050623		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-456321 A 20030606 <--
OTHER SOURCE(S): CASREACT 142:48011
GI



I

AB The present invention provides dipyrrin-substituted porphyrinic macrocycles, intermediates useful for making the same, and methods of making the same. One method to prepare a dipyrrin-substituted porphyrinic macrocycle is by coupling (e.g., Suzuki or Sonogashira coupling) a porphyrinic macrocycle and a bis(dipyrrinato)metal, then demetalating the product with a thiol reagent. A bis(dipyrrinato)metal complex is prepared by reacting a dipyrromethane with an oxidant (e.g., DDQ, o-chloranil, p-chloranil) and a metal salt, which may be performed in a single-pot reaction step. Thus, bis(dipyrrinato)metal complexes I (M = Zn, R = Ph, 4-IC6H4, 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl, 4-OHCC6H4, mesityl, F5C6) were prepared from reaction of the appropriate dipyrromethane with DDQ or p-chloranil and Zn(OAc)2 in 31-86% isolated yield.

Disassembling the bis(dipyrrinato)metal complex to produce sep. dipyrrin groups comprises reacting a bis(dipyrrinato)metal complex with a thiol reagent under neutral conditions. Thus, demetalation of I was achieved by reaction with threo-1,4-dimercapto-2,3-butanediol (DTT) in CH2Cl2 to give free base dipyrrin. A dipyrrin-substituted porphyrinic macrocycle is also prepared by condensing a dipyrromethanedicarbinol with a dipyrrin-substituted dipyrromethane in a weakly polar solvent in the presence of a Lewis acid. The dipyrromethanedicarbinol has at least one covalently attached porphyrinic macrocycle which may be metalated. A trans-(dipyrrin)2-porphyrinic macrocycle is prepared by reacting a dipyrrin-carboxaldehyde with a dipyrromethane in the presence of an acid catalyst. Such compds. and **polymers** of linked **porphyrinic** macrocycles containing dipyrrins may be used for making **mol.** memory **devices**, solar cells and light harvesting arrays.

IC ICM C07F001-08

INCL 548402000

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 27, 28, **35**, 52

ST dipyrrin porphyrin macrocycle prepn; data storage device dipyrrin porphyrin macrocycle; light harvesting array dipyrrin porphyrin macrocycle; transition metal dipyrrin **porphyrin** prepn **polymer**

IT Photosystems
(preparation of dipyrrin-substituted porphyrinic macrocycles for use in light harvesting arrays)

IT Memory devices
(preparation of dipyrrin-substituted porphyrinic macrocycles for use in **mol.** memory **devices**)

IT Metalloporphyrins
Porphyrins
RL: RCT (Reactant); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of dipyrrin-substituted porphyrinic macrocycles for use in **mol.** memory **devices**, solar cells and light harvesting arrays)

IT Solar cells
(preparation of dipyrrin-substituted porphyrinic macrocycles for use in solar cells)

IT **Polymers**, preparation
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(preparation of **polymers** comprised of dipyrrin-substituted **porphyrinic** macrocycles for use in **mol.** memory **devices**, solar cells and light harvesting arrays)

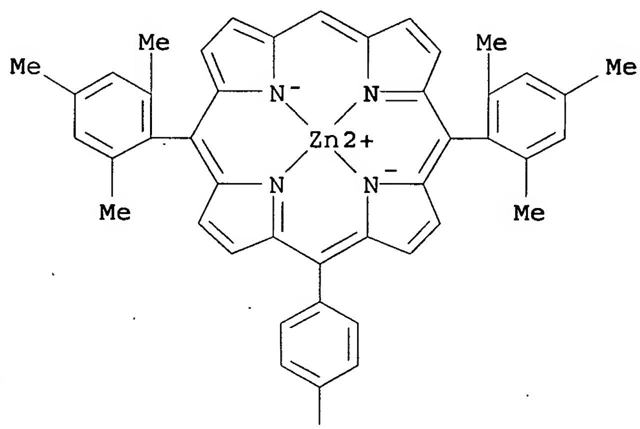
IT 97-94-9, Triethylborane 1493-13-6D, Triflic acid, lanthanide(III) salts 7647-17-8, Cesium chloride, uses 7783-63-3, Titanium tetrafluoride 7784-18-1, Aluminum trifluoride 10025-82-8, Indium trichloride 10099-58-8, Lanthanum trichloride 13450-95-8, Germanium tetraiodide 13465-55-9, Samarium trichloride hexahydrate 19423-80-4, Europium trichloride hydrate 144026-79-9, Scandium(III) triflate
RL: CAT (Catalyst use); USES (Uses)
(Lewis acid; for preparation of dipyrrin-substituted porphyrinic macrocycles from dipyrromethane-dicarbinols)

IT 543-90-8, Cadmium diacetate 7789-48-2, Magnesium dibromide 10043-52-4, Calcium chloride, reactions 10102-05-3, Palladium dinitrate
RL: RCT (Reactant); RACT (Reactant or reagent)
(failed metalation reaction; preparation of dipyrrin-substituted porphyrinic macrocycles for use in data storage devices and light harvesting

arrays)
IT 147804-54-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(failed oxidation/metalation; preparation of dipyrrin-substituted porphyrinic
macrocycles for use in data storage devices and light harvesting
arrays)
IT 3483-12-3, threo-1,4-Dimercapto-2,3-butanediol
RL: RCT (Reactant); RACT (Reactant or reagent)
(for demetalation of bis(dipyrrinato)metal complexes)
IT 84-58-2, DDQ 118-75-2, p-Chloranil, reactions 2435-53-2, o-Chloranil
RL: RGT (Reagent); RACT (Reactant or reagent)
(oxidant; preparation of dipyrrin-substituted porphyrinic macrocycles for
use in data storage devices and light harvesting arrays)
IT 382138-83-2P 807335-91-7P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of dipyrrin-substituted porphyrinic macrocycles for use in data
storage devices and light harvesting arrays)
IT 109-97-7, Pyrrole 142-71-2, Copper diacetate 487-68-3, Mesitaldehyde
557-34-6, Zinc acetate 1571-08-0, Methyl 4-formylbenzoate 3375-31-3,
Palladium diacetate 21211-65-4 25015-63-8, 4,4,5-Tetramethyl-1,3,2-
dioxaborolane 51364-51-3, Tris(dibenzylideneacetone)dipalladium
87199-17-5, 4-Formylphenylboronic acid 155796-90-0 159152-12-2
159152-14-4 167482-91-9 171523-04-9 307930-48-9 307930-58-1
389799-72-8 389799-74-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of dipyrrin-substituted porphyrinic macrocycles for use in data
storage devices and light harvesting arrays)
IT 107798-98-1P 118762-53-1P 167482-98-6P 208191-77-9P 250695-22-8P
286464-42-4P 382138-82-1P 394736-98-2P 630110-82-6P 630110-83-7P
630110-84-8P 630110-86-0P 630110-88-2P 630110-92-8P 630110-93-9P
630110-94-0P 630111-00-1P 630111-04-5P 784151-99-1P 807335-85-9P
807335-86-0P 807335-88-2P 807335-90-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of dipyrrin-substituted porphyrinic macrocycles for use in data
storage devices and light harvesting arrays)
IT 573715-38-5P **630110-95-1P** 630110-96-2P 630110-97-3P
630110-98-4P 630110-99-5P 630111-03-4P
RL: RCT (Reactant); SPN (Synthetic preparation); TEM (Technical or
engineered material use); PREP (Preparation); RACT (Reactant or reagent);
USES (Uses)
(preparation of dipyrrin-substituted porphyrinic macrocycles for use in data
storage devices and light harvesting arrays)
IT 630110-85-9P 630110-87-1P 630110-89-3P 630110-90-6P 807335-82-6P
807335-83-7P 807335-84-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dipyrrin-substituted porphyrinic macrocycles for use in data
storage devices and light harvesting arrays)
IT **630111-05-6P 630111-06-7P 630111-07-8P**
630111-08-9P 807335-89-3P
RL: SPN (Synthetic preparation); TEM (Technical or engineered material
use); PREP (Preparation); USES (Uses)
(preparation of dipyrrin-substituted porphyrinic macrocycles for use in data
storage devices and light harvesting arrays)
IT **630110-95-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); TEM (Technical or
engineered material use); PREP (Preparation); RACT (Reactant or reagent);
USES (Uses)
(preparation of dipyrrin-substituted porphyrinic macrocycles for use in data

storage devices and light harvesting arrays)
RN 630110-95-1 HCAPLUS
CN Palladium, bis[μ-[10-[4-[(1H-pyrrol-2-yl-κN)(2H-pyrrol-2-ylidene-κN)methyl]phenyl]-5,15-bis(2,4,6-trimethylphenyl)-21H,23H-porphinato(3-)-κN21,κN22,κN23,κN24]]bis(zinc)-
(9CI) (CA INDEX NAME)

PAGE 1-A



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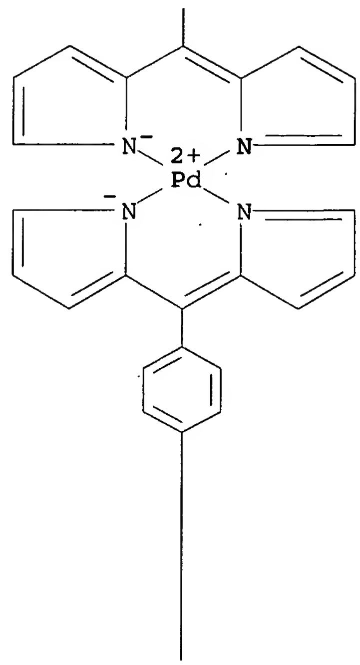

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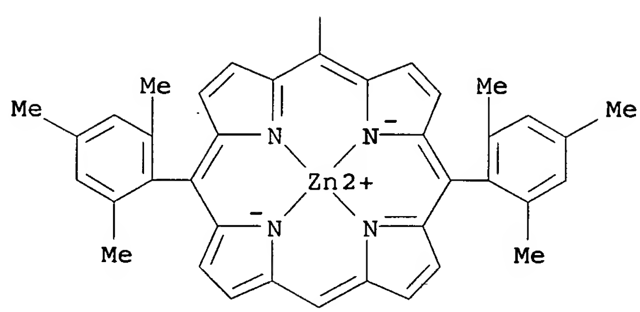


L47 ANSWER 4 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:330227 HCAPLUS
DOCUMENT NUMBER: 140:367250
TITLE: **Molecular device**, **molecular** assembly, rectifier, rectifying method, sensor, switching device, circuit device, logical circuit device, operational device, and information processing device
INVENTOR(S): Oda, Masao; Matsumura, Hiroshi
PATENT ASSIGNEE(S): Sony Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 28 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
JP 2004123720	A2	20040422	JP 2003-279955		20030725	<--
CN 1495908	A	20040512	CN 2003-125570		20030911	<--
US 2004094818	A1	20040520	US 2003-660098		20030911	<--
US 6914276	B2	20050705				
US 2005175984	A1	20050811	US 2005-100202		20050406	<--
US 2005205895	A1	20050922	US 2005-100156		20050406	<--
PRIORITY APPLN. INFO.:			JP 2002-265924	A	20020911	<--
			JP 2003-279955	A	20030725	<--
			US 2003-660098	A1	20030911	<--

AB A **mol. device** has rectifier function which gives off transfer of excitation state or excitons asym. The excitation state or excitons may be formed or generated by giving a stimulus to the device from the outside such as light, or the excitation state or excitons generated outside may be injected to the device, or these methods may be combined. The mol. assemblies may comprise linear conjugated **polymers**, linear nonconjugated **polymers**, or linear mol. assocs. composed of mols. of same or different types. In another alternative, the mol. assemblies may comprise circular or oval mols. or mol. assemblies composed of circular conjugated **polymers**, circular nonconjugated **polymers**, or circular mol. assocs. composed of mols. of same or different types. The mols. or mol. assemblies are phys. or chemical bonded by conjugated bonds, nonconjugated bonds, charge-transfer bonding, ionic bonds, hydrogen bonds, stacking by interaction of π electrons, van der Waars force, or intermediary force of these. By controlling the rectifier function, an ion sensor or a switching device is formed. Transfer of excitation state or excitons from one mol. or mol. assembly to another bonding mol. or assembly takes place asym. because of spacial asymmetry at the bonding point, thereby obtaining the rectifier function. A resistor may be inserted in the middle of the rectifier. The resistor may comprise mols. or mol. assemblies bonding to mols. or mol. assemblied of the **mol. devices** by covalent bonds. The structure of the mols. or mol. assemblies of the resistor may be changed by electromagnetic wave irradiation or by temperature
The
mol. device may be provided with ≥1 input terminals in ≥1 of mols. or mol. assemblies. The input terminal may inputs the excitation states or excitons to the **mol. devices** by photoinduced surface plasmon excitation. The input terminal may be prepared by modification of an end of the mols. or mol. assemblies with colorant mols. having desired MO energy. The rectifier function is applied to a sensor device and a switching device for a circuit device, a logical circuit device, an operational device, and an information processing device. Preferably, ≥1 of mols. or mol. assemblies have ion detection function.

IC ICM C07D519-00
ICS H01L029-06; H01L029-66; H01L051-00; C07F003-06

CC 76-14 (Electric Phenomena)
Section cross-reference(s): 28, 29

ST **mol device** rectifier sensor switch; circuit **device mol** rectifier; logical circuit **device mol** rectifier; operational **device mol** rectifier; information processing **device mol** rectifier

IT Coloring materials
(modification of mols. with, for input terminal; **mol. device** and **mol.** assembly having rectifier function

and its application)

IT Computers
Electrooptical switches
Energy transfer
Exciton
Integrated circuits
Molecules
Rectifiers
Resistors
Self-assembly
Sensors
(**mol. device** and **mol.** assembly having rectifier function and its application)

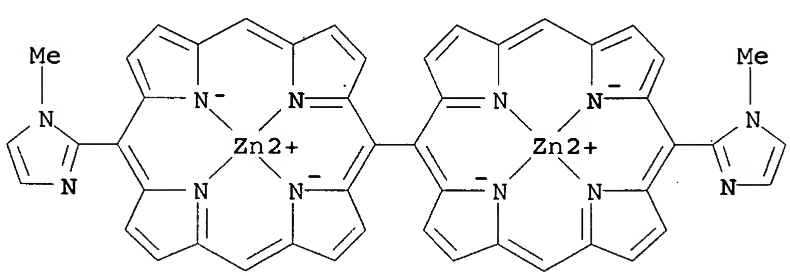
IT 101-60-0D, 21H,23H-Porphine, derivs., **polymers** 14052-02-9D, allyl or alkyl derivs. **681427-87-2** **681427-88-3** **681427-89-4** 681427-90-7D, derivs. **681427-91-8**
RL: DEV (Device component use); USES (Uses)
(**mol. device** and **mol.** assembly having rectifier function and its application)

IT 71-43-2, Benzene, uses 103-33-3, Azobenzene
RL: DEV (Device component use); USES (Uses)
(resistor; **mol. device** and **mol.** assembly having rectifier function and its application)

IT **681427-87-2**
RL: DEV (Device component use); USES (Uses)
(**mol. device** and **mol.** assembly having rectifier function and its application)

RN 681427-87-2 HCAPLUS

CN Zinc, [μ-[15,15'-bis(1-methyl-1H-imidazol-2-yl)-5,5'-bi-21H,23H-porphinato(4-)-κN21,κN22,κN23,κN24:κN21',.ka ppa.N22',κN23',κN24']]di- (9CI) (CA INDEX NAME)



L47 ANSWER 5 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:52150 HCAPLUS
DOCUMENT NUMBER: 140:393275
TITLE: Photoelectrochemical properties of supramolecular species containing porphyrin and ruthenium complexes on TiO2 films
AUTHOR(S): Nogueira, Ana F.; Formiga, Andre Luiz B.; Winnischofer, Herbert; Nakamura, Marcelo; Engelmann, Fabio M.; Araki, Koiti; Toma, Henrique E.
CORPORATE SOURCE: Instituto de Quimica - Universidade de Sao Paulo, Sao Paulo, 05513-970, Brazil
SOURCE: Photochemical & Photobiological Sciences (**2004**), 3(1), 56-62
CODEN: PPSHCB; ISSN: 1474-905X

PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Modification of wide band gap semiconductor surfaces by a new generation of supramol. sensitizers, combining porphyrin and ruthenium-phenanthroline complexes leads to versatile mol. interfaces, allowing the exploitation of photoinduced charge transfer in dye sensitized photoelectrochem. cells. Meso-Tetrapyridylporphyrin coordinated to two ruthenium complexes converts 21% of the incident photons into current after excitation at the Soret band. The authors discuss the electron/energy transfer mechanisms involved in the TiO_2 sensitization by these supramol. species, invoking some theor. calcns. Two ruthenium complexes (photosensitizing dyes containing 2 or 4 ruthenium 1,10-phenanthroline groups) were synthesized, characterized, and nanoporous TiO_2 films were treated with the dyes. Heterojunction solar cells were assembled with t-butylpyridine, tetrabutylammonium iodide, and iodine electrolyte, dye:TiO_2 coated SnO_2:F- glass ad platinum-doped SnO_2:F- glass, separated by PVC film. Absorption and emission spectra of the dye were compared with mol. modeling calcns. of energy levels. Atomic force microscope images ensured effective dye penetration into the TiO_2 film. Photon-to-electron conversion efficiency curves (IPCE) vs. λ were measured and resemble the absorption spectra of the dyes. The current-potential relationship for cells prepared with the Ru2phenTPyP dye. The 4-ruthenium group cell showed negligible photocurrent, <2% IPCE.

CC 52-2 (Electrochemical, Radiational, and Thermal Energy Technology)
Section cross-reference(s): 27, 72, **73**, 76

ST photosensitizing dye supramol porphyrin ruthenium phenanthroline complex titania film; heterojunction solar cell mol modeling energy level absorption spectra; photoelectrochem photocurrent energy transfer solar cell ruthenium iodide electrolyte

IT Solar energy
(conversion; photoelectrochem. properties of supramol. species containing porphyrin and ruthenium complexes on TiO_2 films)

IT Band gap
Electric current-potential relationship
Emission spectra
HOMO (molecular orbital)
Heterojunction solar cells
IR spectra
LUMO (molecular orbital)
Molecular modeling
Photocurrent
UV and visible spectra
(photoelectrochem. properties of supramol. species containing porphyrin and ruthenium complexes on TiO_2 films)

IT Dyes
(photosensitizing; photoelectrochem. properties of supramol. species containing porphyrin and ruthenium complexes on TiO_2 films)

IT Glass **substrates**
(tin dioxide-coated; photoelectrochem. properties of supramol. species containing porphyrin and ruthenium complexes on TiO_2 films)

IT 18282-10-5, Tin dioxide
RL: **DEV (Device component use)**; EPR (Engineering process); PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process); USES (Uses)
(F- doped; photoelectrochem. properties of supramol. species containing porphyrin and ruthenium complexes on TiO_2 films)

IT 7782-41-4, Fluorine, uses
RL: **DEV (Device component use)**; EPR (Engineering process); PEP (Physical, engineering or chemical process); PYP (Physical process); PROC

(Process); USES (Uses)
(SnO2 doped with; photoelectrochem. properties of supramol. species containing porphyrin and ruthenium complexes on TiO2 films)

IT 311-28-4, Tetrabutylammonium iodide 2567-83-1, Tetraethylammonium perchlorate 7553-56-2, Iodine, uses 118676-08-7, tert-Butylpyridine
RL: **DEV (Device component use)**; USES (Uses)
(photoelectrochem. properties of supramol. species containing porphyrin and ruthenium complexes on TiO2 films)

IT 9002-86-2, Polyvinyl chloride 13463-67-7, Titanium oxide (TiO2), uses
RL: **DEV (Device component use)**; EPR (Engineering process); PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process); USES (Uses)
(photoelectrochem. properties of supramol. species containing porphyrin and ruthenium complexes on TiO2 films)

IT 7440-06-4P, Platinum, uses
RL: **DEV (Device component use)**; EPR (Engineering process); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); USES (Uses)
(photoelectrochem. properties of supramol. species containing porphyrin and ruthenium complexes on TiO2 films)

IT **214971-88-7P 686348-41-4P 686348-43-6P**
RL: **DEV (Device component use)**; PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); PYP (Physical process); SPN (Synthetic preparation); **PREP (Preparation)**; PROC (Process); USES (Uses)
(photoelectrochem. properties of supramol. species containing porphyrin and ruthenium complexes on TiO2 films)

IT **214971-88-7P**
RL: **DEV (Device component use)**; PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); PYP (Physical process); SPN (Synthetic preparation); **PREP (Preparation)**; PROC (Process); USES (Uses)
(photoelectrochem. properties of supramol. species containing porphyrin and ruthenium complexes on TiO2 films)

RN 214971-88-7 HCAPLUS
CN Ruthenium(4+), tetrachlorooctakis(1,10-phenanthroline-κN1,κN10)[μ4-[5,10,15,20-tetra(4-pyridinyl-κN)-21H,23H-porphine]]tetra-, salt with trifluoromethanesulfonic acid (1:4) (9CI) (CA INDEX NAME)

CM 1

CRN 214971-87-6
CMF C136 H90 Cl4 N24 Ru4
CCI CCS

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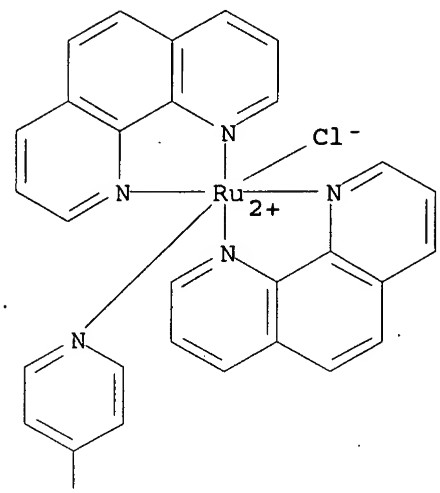

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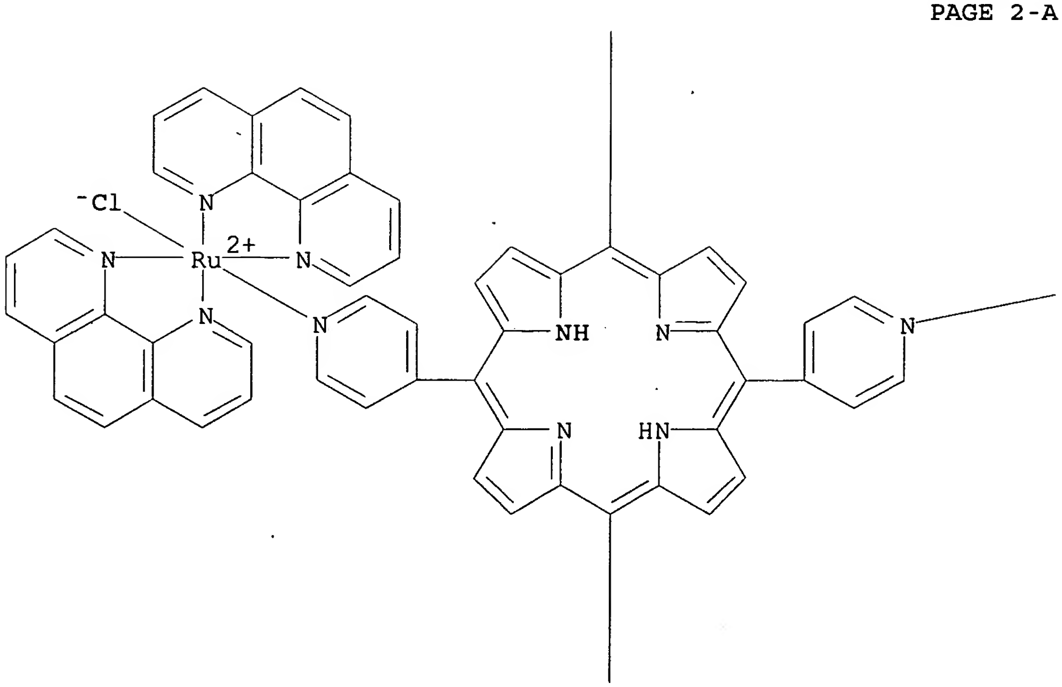

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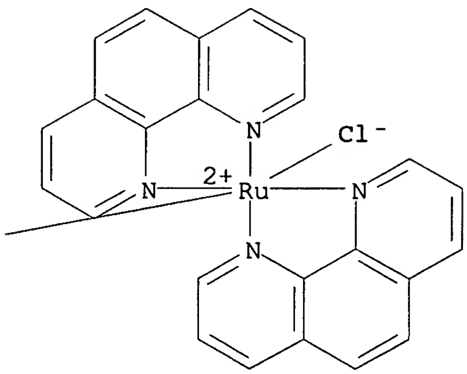

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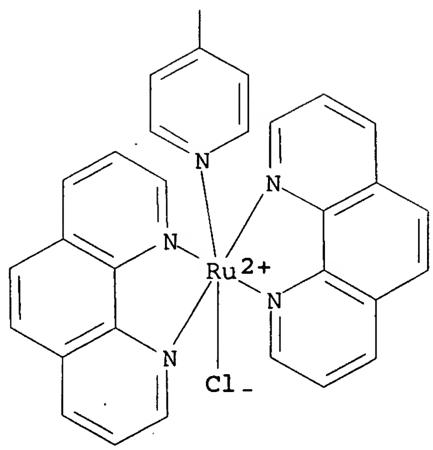
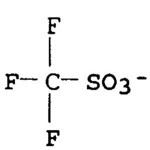


CM 2

CRN 37181-39-8
CMF C F3 O3 S



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 6 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:42427 HCAPLUS
DOCUMENT NUMBER: 140:270451

TITLE: Encapsulation of Transition Metal Catalysts by Ligand-Template Directed Assembly

AUTHOR(S): Slagt, Vincent F.; Kamer, Paul C. J.; Van Leeuwen, Piet W. N. M.; Reek, Joost N. H.
CORPORATE SOURCE: Hoff Institute of Molecular Sciences, University of Amsterdam, Amsterdam, 1018 WV, Neth.

SOURCE: Journal of the American Chemical Society (**2004**), 126(5), 1526-1536
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:270451

AB Encapsulated transition metal catalysts are presented that are formed by templated self-assembly processes of simple building blocks such as porphyrins and pyridylphosphine and phosphite ligands, using selective metal-ligand interactions. These ligand assemblies coordinate to transition metals, leading to a new class of transition metal catalysts. The assembled catalyst systems were characterized using NMR and UV-visible spectroscopy and were identified under catalytic conditions using high-pressure IR spectroscopy. Tris-3-pyridylphosphine binds three mesophenyl Zn(II) porphyrin units and consequently forms an assembly with the P donor atom completely encapsulated. The encapsulated phosphines lead exclusively to monoligated transition metal complexes, and in the Rh-catalyzed hydroformylation of 1-octene the encapsulation of the catalysts resulted in a 10-fold increase in activity. The branched aldehyde was formed preferentially (l/b = 0.6), a selectivity that is highly unusual for this **substrate**, which is attributed to the encapsulation of the transition metal catalysts. An encapsulated Rh catalyst based on Ru(II) porphyrins and tris-meta-pyridyl phosphine resulted in an even larger selectivity for the branched product (l/b = 0.4). These encapsulated catalysts can be prepared easily, and various template ligands and porphyrins, such as tris-3-pyridyl phosphite and Ru(II) porphyrins, were explored, leading to catalysts with different properties.

CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 29, 67, **73**, 78

ST encapsulation transition metal catalyst ligand template

IT Transition metal complexes
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(aryl porphyrin complexes; encapsulation of transition metal catalysts by ligand-template directed assembly)

IT Porphyrins
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(aryl, transition metal complexes; encapsulation of transition metal catalysts by ligand-template directed assembly)

IT Aldehydes, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(branched favored over linear; encapsulation of transition metal catalysts by ligand-template directed assembly)

IT Complexation
Encapsulation
Formation constant
Hydroformylation
Hydroformylation catalysts
Hydroformylation kinetics

Molecular modeling
PM3 (molecular orbital method)
Self-assembly
Supramolecular structure
Synthesis gas
UV and visible spectra
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT Transition metal complexes
RL: CAT (Catalyst use); USES (Uses)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT Carbonyl complexes
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT Ligands
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT IR spectra
IR spectroscopy
(high-pressure in-situ; encapsulation of transition metal catalysts by ligand-template directed assembly)

IT Cooperative phenomena
(in ligand binding to transition metal; encapsulation of transition metal catalysts by ligand-template directed assembly)

IT Chelation
(template; encapsulation of transition metal catalysts by ligand-template directed assembly)

IT Steric hindrance
(to ligand coordination; encapsulation of transition metal catalysts by ligand-template directed assembly)

IT NMR (nuclear magnetic resonance)
(1H; encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 7786-29-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(catalyst for preparation of; encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 111-67-1P, 2-Octene 592-98-3P, 3-Octene 592-99-4P, 4-Octene
RL: BYP (Byproduct); PREP (Preparation)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 644966-12-1 **673485-16-0** 673485-17-1 673485-18-2
673485-19-3 673485-20-6 673485-21-7
673485-22-8 673485-23-9 674291-55-5
RL: CAT (Catalyst use); CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 673485-15-9
RL: CAT (Catalyst use); CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT

(Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 14074-80-7, Zinc tetraphenylporphyrin 32073-84-0
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 673455-61-3P
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 14874-82-9 94345-02-5
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 603-35-0, Triphenylphosphine, reactions 54750-98-0 104114-99-0 164080-49-3
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT **673485-03-5P 673485-04-6P**
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 110-86-1, Pyridine, reactions 111-66-0, 1-Octene
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 630-08-0, Carbon monoxide, reactions 14220-64-5, Palladium, bis(benzonitrile)dichloro-
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT **673485-05-7 673485-09-1** 673485-13-7
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 673485-11-5
RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 109-00-2, 3-Hydroxypyridine 557-34-6, Zinc acetate 4422-95-1, 1,3,5-Benzenetricarbonyl trichloride 7719-12-2, Phosphorus trichloride 63936-85-6 110275-59-7 673485-07-9
RL: RCT (Reactant); RACT (Reactant or reagent)

(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 673485-02-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT 124-19-6P, Nonanal

RL: SPN (Synthetic preparation); PREP (Preparation)

(encapsulation of transition metal catalysts by ligand-template directed assembly)

IT **673485-16-0**

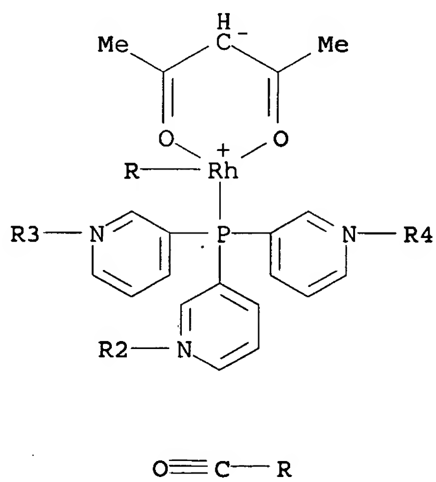
RL: CAT (Catalyst use); CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent); USES (Uses)

(encapsulation of transition metal catalysts by ligand-template directed assembly)

RN 673485-16-0 HCAPLUS

CN Rhodium, carbonyl(2,4-pentanedionato-κO,κO')[μ4-[3,3',3''-(phosphinidyne-κP)tris[pyridine-κN]]]tris[[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-κN21,κN22,κN23,.kappa .N24]zinc]- (9CI) (CA INDEX NAME)

PAGE 1-A



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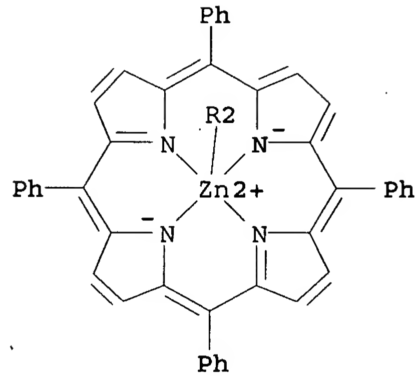

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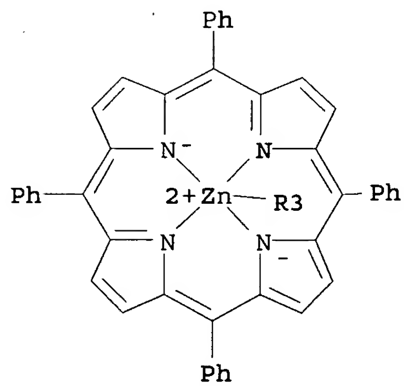

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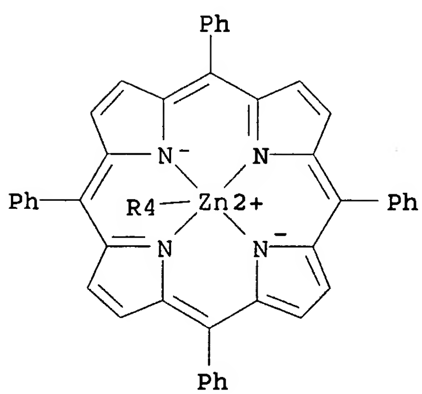


REFERENCE COUNT: 182 THERE ARE 182 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L47 ANSWER 7 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:954896 HCAPLUS
DOCUMENT NUMBER: 140:171859
TITLE: Organic light emitting diodes and photo detectors fabricated on a **polymeric substrate** for flexible optical integrated **devices**
AUTHOR(S): Ohmori, Yutaka; Kajii, Hirotake; Taneda, Takayuki; Kaneko, Masamitsu
CORPORATE SOURCE: Collaborative Research Center for Advanced Science and Technology (CRCAST), Osaka University, Osaka, 565-0871, Japan
SOURCE: Materials Research Society Symposium Proceedings (**2003**), 769(Flexible Electronics--Materials and Device Technology), 131-140
CODEN: MRSPDH; ISSN: 0272-9172
PUBLISHER: Materials Research Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Direct fabrication of organic light emitting diodes (OLED) on a **polymeric substrate**, i.e., **polymeric** waveguide **substrate** to form a flexile optical integrated **devices** was realized. The OELD was fabricated by organic mol. beam deposition (OMBD) technique on a **polymeric substrate** and a glass **substrate**, for comparison. The **device** fabricated on a **polymeric substrate** shows similar **device** characteristics to that on a glass substrate. Optical signal of faster than 100 MHz was created by applying pulsed voltage directly to the OLED with emissive layers using rubrene or porphine doped in 8-hydroxyquinoline Al derivs. Optical signal transmission with OLED fabricated on a **polymeric** waveguide with optical connectors was successfully realized. Optical photo detectors (OPD) using phthalocyanine derivs. with superlattice structure provide increased pulse response with input optical signals, and the OPD with 5 MHz of cut-off frequency was realized with superlattice structure under reverse bias voltage to the OPD.

CC 73-11 (**Optical**, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): **36**, 76

ST integrated LED photodetector org substrate glass polyimide; detector optical integrated LED org substrate glass polyimide

IT Electroluminescent **devices**
(blue-emitting; organic LEDs and photodetectors fabricated on **polymeric substrate** for flexible optical integrated **devices**)

IT Electroluminescent **devices**
(green-emitting; organic LEDs and photodetectors fabricated on **polymeric substrate** for flexible optical integrated **devices**)

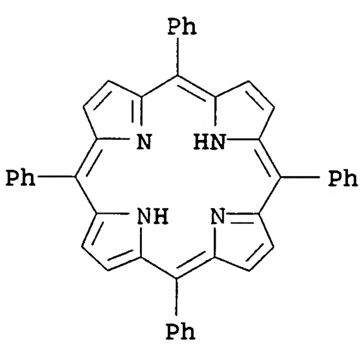
IT Electric current-potential relationship
(of organic photodetectors fabricated on **polymer substrate** for flexible optical integrated **devices**)

IT Glass substrates
(organic LEDs and photodetectors fabricated on glass substrate for flexible optical integrated **devices**)

IT Optical detectors
Optical integrated circuits
(organic LEDs and photodetectors fabricated on **polymeric substrate** for flexible optical integrated **devices**)

IT Polyimides, uses

RL: **DEV (Device component use)**; USES (Uses)
(substrates; organic LEDs and photodetectors fabricated on **polymer substrate** for flexible optical integrated **devices**)
IT Electroluminescent **devices**
(thin-film; organic LEDs and photodetectors fabricated on **polymeric substrate** for flexible optical integrated **devices**)
IT 517-51-1, Rubrene **917-23-7**, 5,10,15,20-Tetraphenyl-21H,23H-porphine
RL: **DEV (Device component use)**; MOA (Modifier or additive use); USES (Uses)
(hydroxyquinoline aluminum containing; organic LEDs and photodetectors fabricated on **polymer substrate** for flexible optical integrated **devices** containing)
IT 2085-33-8, 8-Hydroxyquinoline aluminum 4733-39-5, 2,9-Dimethyl-4,7-diphenyl-1,10-phenanthroline 7631-86-9, Silica, uses 12033-89-5, Silicon nitride, uses 14916-87-1 26201-32-1, Titanyl phthalocyanine 31396-84-6 50926-11-9, ITO 83054-80-2, N,N'-Bis(2,5-di-tert-butylphenyl)-3,4,9,10-perylene-dicarboximide 123847-85-8, α-NPD
RL: **DEV (Device component use)**; USES (Uses)
(organic LEDs and photodetectors fabricated on **polymer substrate** for flexible optical integrated **devices** containing)
IT **917-23-7**, 5,10,15,20-Tetraphenyl-21H,23H-porphine
RL: **DEV (Device component use)**; MOA (Modifier or additive use); USES (Uses)
(hydroxyquinoline aluminum containing; organic LEDs and photodetectors fabricated on **polymer substrate** for flexible optical integrated **devices** containing)
RN 917-23-7 HCAPLUS
CN 21H,23H-Porphine, 5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 8 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:884635 HCAPLUS
DOCUMENT NUMBER: 140:66909
TITLE: Transient Absorption Studies of the Pacman Effect in Spring-Loaded Diiron(III) μ-Oxo Bisporphyrins
AUTHOR(S): Hodgkiss, Justin M.; Chang, Christopher J.; Pistorio, Bradford J.; Nocera, Daniel G.
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139-4307, USA
SOURCE: Inorganic Chemistry (**2003**), 42(25),

8270-8277
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Picosecond transient absorption spectroscopy of diiron(III) μ-oxo bisporphyrins appended to xanthene, (DPX)Fe2O and (DPXM)Fe2O, and dibenzofuran (DPD)Fe2O have been investigated in order to decipher the effect of a spring-loaded cleft on their photophysics and attendant oxidation photocatalysis. The tension of the cofacial pocket is systematically tuned with the bridge span and meso-substitution opposite to the bridge; the distances of the relaxed cofacial pockets and clamped Fe-O-Fe pockets are known from X-ray crystallog. (ΔdM-M(relaxed - clamped) = 4.271 Å (DPD), 2.424 Å (DPXM), 0.208 Å (DPX)). The photophys. and chemical properties of these cofacial platforms are compared to the unbridged diiron(III) μ-oxo analog, (Etio)2Fe2O. Photon absorption by the diiron(III) μ-oxo chromophore prompts Fe-O-Fe photocleavage to release the spring and present a PFeIVO/PFeII pair (P = porphyrin subunit); net photooxidn. is observed when oxygen atom transfer to **substrate** occurs before the spring can reclamp to form the μ-oxo species. The inherent lifetimes of the PFeIVO/PFeII pairs for the four compds. are surprisingly similar (τ[(DPD)Fe2O] = 1.36(3) ns, τ[(DPX)Fe2O] = 1.26(5) ns, τ[(DPXM)Fe2O] = 1.27(9) ns, and τ[(Etio)2Fe2O] = 0.97(3) ns), considering the structural differences arising from tensely clamped (DPD and DPXM), relaxed (DPX), and unbridged (Etio) cofacial architectures. However, the rates of net oxygen atom transfer for (DPD)Fe2O and (Etio)2Fe2O are found to be 4 orders of magnitude greater than that of (DPX)Fe2O and 2 orders of magnitude greater than that of (DPXM)Fe2O. These results show that the spring action of the cleft, known as the Pacman effect, does little to impede reclamping to form the μ-oxo species but rather is manifest to opening the cofacial cleft to allow **substrate** access to the photogenerated oxidant. Consistent with this finding, photooxidn. efficiencies decrease as the steric demand of **substrates** increase.

CC 73-4 (**Optical**, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 9, 22, 67, 78

ST transient absorption spectrum Pacman effect iron oxo bisporphyrin; structure function relationship iron oxo bisporphyrin

IT Porphyrins
RL: PRP (Properties)
(bisporphyrins, bridged; transient absorption studies of Pacman effect in spring-loaded diiron-oxo bisporphyrins)

IT Molecular structure-property relationship
(of spring-loaded diiron-oxo bisporphyrins)

IT Oxidation, photochemical
(of spring-loaded diiron-oxo bisporphyrins in relation to structure)

IT Catalysts
(photochem.; of spring-loaded diiron-oxo bisporphyrins in relation to structure)

IT Tension
(transient absorption studies of Pacman effect in spring-loaded diiron-oxo bisporphyrins)

IT UV and visible spectra
(transient; of spring-loaded diiron-oxo bisporphyrins)

IT **54348-75-3**
RL: NUU (Other use, unclassified); PRP (Properties); USES (Uses)
(transient absorption studies of Pacman effect in spring-loaded diiron-oxo bisporphyrins)

IT **259669-12-0 442197-53-7**

RL: PRP (Properties)
(transient absorption studies of Pacman effect in spring-loaded diiron-oxo bisporphyrins)

IT **54348-75-3**
RL: NUU (Other use, unclassified); PRP (Properties); USES (Uses)
(transient absorption studies of Pacman effect in spring-loaded diiron-oxo bisporphyrins)

RN 54348-75-3 HCAPLUS

CN Iron, μ-oxobis[2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 9 OF 56 HCAPLUS

ACCESSION NUMBER: 2003:884634 HCAPLUS
DOCUMENT NUMBER: 140:86509

TITLE: The Pacman effect: a supramolecular strategy for controlling the excited-state dynamics of pillared cofacial bisporphyrins

AUTHOR(S): Chang, Christopher J.; Loh, Zhi-Heng; Deng, Yongqi; Nocera, Daniel G.
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139-4307, USA

SOURCE: Inorganic Chemistry (**2003**), 42(25), 8262-8269
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:86509

AB The mol. recognition properties of dizinc(II) bisporphyrin anchored by dibenzofuran (DPD), Zn2(DPD) (1), were evaluated as a strategy for using the Pacman effect to control the excited-state properties of cofacial bisporphyrin motifs. Crystallog. studies establish that DPD furnishes a cofacial system with vertical flexibility and horizontal preorganization. The structure determination of a **substrate**-bound DPD species, Zn2(DPD)(2-aminopyrimidine) (2), completes a set of structurally homologous Zn(II) porphyrin host and host-guest complexes, which offer a direct structural comparison for the Pacman effect upon **substrate** complexation. Binding studies reveal that pyrimidine encapsulation by the DPD framework is accompanied by a markedly reduced entropic penalty (.apprx.60 J mol-1K-1) with respect to traditional face-to-face bisporphyrin systems, giving rise to a smaller conformational energy cost upon **substrate** binding. Transient absorption spectroscopy reveals that **substrate** encapsulation within the DPD cleft dramatically affects excited-state dynamics of cofacial bisporphyrins. The emission lifetime of host-guest complex 2 increases by more than an order of magnitude compared to free host 1. In the absence of the guest, the excited-state dynamics are governed by torsional motion of the porphyrin rings about the aryl ring of the DPD pillar. Host-guest binding attenuates this conformational flexibility, thereby removing efficient nonradiative decay pathways. Taken together, these findings support the exceptional ability of the DPD system to structurally accommodate reaction intermediates during catalytic turnover and provide a novel supramol. approach toward developing a reaction chemical derived directly from the excited states of Pacman constructs.

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 68, 69, **73**, 75
ST zinc porphyrin aminopyrimidine complex prepn structure; crystal structure zinc bisporphyrin aminopyrimidine complex; assocn const zinc bisporphyrin complex pyrimidine; excited state dynamics zinc porphyrin complex
IT Formation constant
(binding consts.; of zinc bisporphyrin complex with pyrimidines)
IT Excited state
(lifetime; of zinc porphyrin complexes)
IT Crystal structure
Formation enthalpy
Formation entropy
Molecular structure
(of zinc bisporphyrin aminopyrimidine complex)
IT UV and visible spectra
(of zinc porphyrin complexes)
IT Molecular structure
(optimization; of zinc bisporphyrin complex with aminopyrimidine from DFT calcns. in relation to stability of zinc bisporphyrin aminopyrimidine complex)
IT 289-95-2, Pyrimidine 591-55-9, 5-Aminopyrimidine 1722-12-9, 2-Chloropyrimidine 4595-60-2, 2-Bromopyrimidine
RL: PRP (Properties)
(binding constant with zinc bisporphyrin complex)
IT 17632-18-7, (Octaethylporphyrinato)zinc 131354-06-8 **261724-78-1**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(excited state lifetime of)
IT **640725-99-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
IT **640725-98-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and excited state lifetime and association constant and optimized
mol. structure of)
IT 109-12-6, 2-Aminopyrimidine
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of zinc bisporphyrin aminopyrimidine complex and binding constant with zinc bisporphyrin complex)
IT **259669-11-9P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(reactant for preparation of zinc bisporphyrin aminopyrimidine complex and excited state lifetime of)
IT **261724-78-1**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(excited state lifetime of)
RN 261724-78-1 HCAPLUS
CN Zinc, [μ-[[5,5'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[2,8,13,17-tetraethyl-3,7,12,18-tetramethyl-21H,23H-porphinato-κN21,κN22,κN23,κN24]](4-)]]di- (9CI) (CA INDEX NAME)

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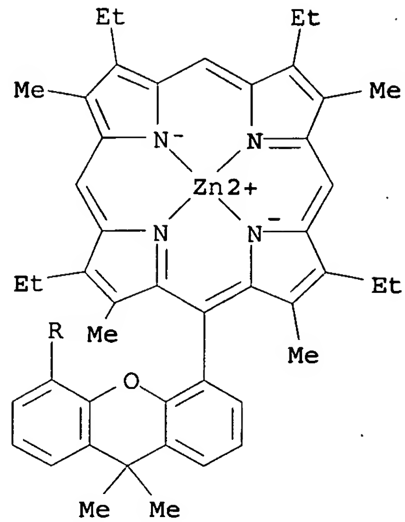

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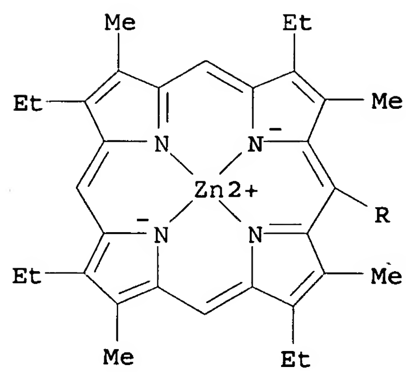


REFERENCE COUNT: 79 THERE ARE 79 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 10 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:753344 HCAPLUS
DOCUMENT NUMBER: 139:395499
TITLE: Magnesium Tetraarylporphyrin Tweezer: a CD-Sensitive Host for Absolute Configurational Assignments of α-Chiral Carboxylic Acids
AUTHOR(S): Proni, Gloria; Pescitelli, Gennaro; Huang, Xuefei; Nakanishi, Koji; Berova, Nina
CORPORATE SOURCE: Department of Chemistry, Columbia University, New York, NY, 10027, USA
SOURCE: Journal of the American Chemical Society (2003), 125(42), 12914-12927
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:395499

AB A protocol to determine the absolute configuration of α-chiral carboxylic acids based on a modified circular dichroic (CD) exciton chirality method has been developed. The protocol relies on a host-guest complexation mechanism: the chiral **substrates** are derivatized to give bifunctional amide conjugates ("guests") that form complexes with a dimeric magnesium porphyrin host, Mg-T (T stands for "tweezer") that acts as a "receptor". The two porphyrins in the complex adopt a preferred helicity dictated by the substituents at the chiral center in accordance with their steric sizes (assigned on the basis of conformational energy A-values) and, consequently, with the absolute configuration of the **substrates** under investigation. This chiroptical method, verified with a variety of chiral **substrates**, has been demonstrated to be reliable and generally applicable, including natural products with complex structures. Mol. modeling, NMR, and FTIR expts. of selected host-guest complexes revealed the mode of ligation of the **substrates** to the magnesium porphyrin species and led to clarification of the structure of the complex. When oxygen functionalities were directly attached to the chiral center, the signs of the CD couplets were opposite to those predicted on the basis of steric size. NMR and mol. modeling expts. indicated that this apparent inconsistency was due to conformational characteristics of the guest mols. The stereochem. anal. is shown to be a sensitive technique, not only for the determination of absolute configurations of
substrates but also for elucidation of their solution conformations.

CC 22-3 (Physical Organic Chemistry)
Section cross-reference(s): **73**, 77, 78

ST magnesium tetraarylporphyrin Tweezer CD abs configuration chiral carboxylic acid

IT Conformation
(helicity; titration and CD spectroscopy on binding constant with host magnesium tetraarylporphyrin tweezer and absolute configuration of α-chiral carboxylic acids)

IT Absolute configuration
Inclusion reaction
Simulation and Modeling
Solvatochromism
Solvent effect
(titration and CD spectroscopy on binding constant with host magnesium tetraarylporphyrin tweezer and absolute configuration of α-chiral carboxylic acids)

IT Porphyrins
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(titration and CD spectroscopy on binding constant with host magnesium tetraarylporphyrin tweezer and absolute configuration of α-chiral carboxylic acids)

IT 68-95-1 302-97-6 514-10-3 611-71-2 1730-91-2 3966-32-3 7782-24-3 13490-69-2 17257-71-5 17407-55-5 18667-97-5 21461-84-7 22204-53-1 29617-66-1 32644-15-8 51146-56-6 53174-06-4 87392-05-0 88335-94-8 106927-66-6 164229-88-3 357396-04-4 479627-34-4 625854-64-0 626243-58-1
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(titration and CD spectroscopy on binding constant with host magnesium tetraarylporphyrin tweezer and absolute configuration of α-chiral carboxylic acids)

IT **626203-52-9 626203-53-0 626203-54-1**
626203-55-2 626203-56-3

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(titration and CD spectroscopy on binding constant with host magnesium tetraarylporphyrin tweezer and absolute configuration of α-chiral carboxylic acids)

IT 625854-40-2P 625854-44-6P 625854-45-7P 625854-56-0P **626203-51-8P** 684215-92-7P 684216-27-1P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(titration and CD spectroscopy on binding constant with host magnesium tetraarylporphyrin tweezer and absolute configuration of α-chiral carboxylic acids)

IT 625854-37-7P 625854-38-8P 625854-39-9P 625854-41-3P 625854-42-4P 625854-43-5P 625854-46-8P 625854-47-9P 625854-48-0P 625854-49-1P 625854-50-4P 625854-51-5P 625854-52-6P 625854-53-7P 625854-54-8P 625854-55-9P 625854-57-1P 625854-58-2P 625854-59-3P 625854-60-6P 625854-61-7P 625854-62-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(titration and CD spectroscopy on binding constant with host magnesium tetraarylporphyrin tweezer and absolute configuration of α-chiral carboxylic acids)

IT 111-29-5, 1,5-Pentanediol 75178-96-0 119730-06-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(titration and CD spectroscopy on binding constant with host magnesium tetraarylporphyrin tweezer and absolute configuration of α-chiral carboxylic acids)

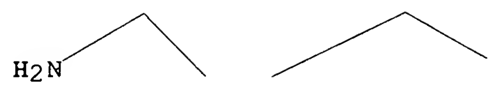
IT 95051-10-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(titration and CD spectroscopy on binding constant with host magnesium tetraarylporphyrin tweezer and absolute configuration of α-chiral carboxylic acids)

IT **626203-52-9**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(titration and CD spectroscopy on binding constant with host magnesium tetraarylporphyrin tweezer and absolute configuration of α-chiral carboxylic acids)

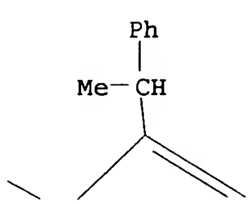
RN 626203-52-9 HCAPLUS

CN Magnesium, [μ-[(αS)-N-[3-(amino-κN)propyl]-α-methylbenzeneacetamide-κO]][μ-[[1,5-pentanediyl bis[4-(10,15,20-triphenyl-21H,23H-porphin-5-yl-κN21,κN22,κN23,κN24)benzoato]](4-)]]di- (9CI) (CA INDEX NAME)

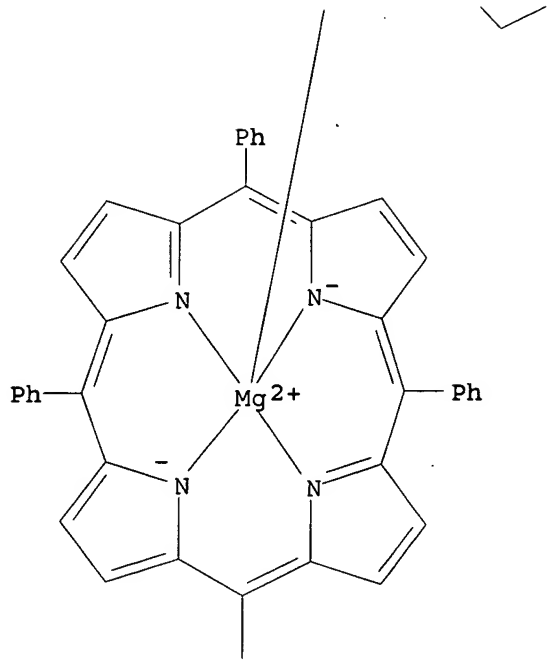
PAGE 1-A



PAGE 1-B



PAGE 2-A



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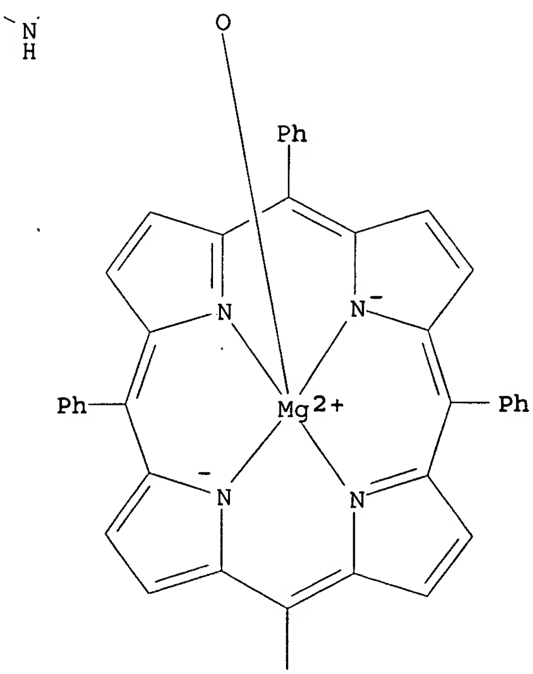
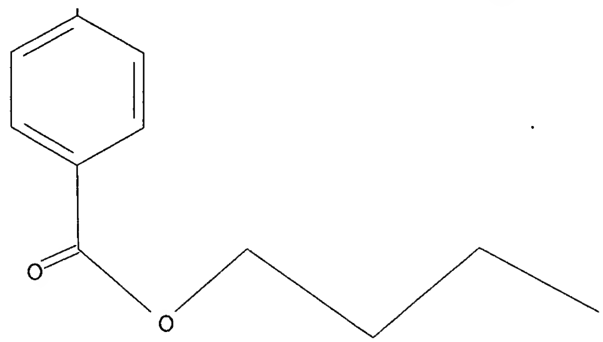
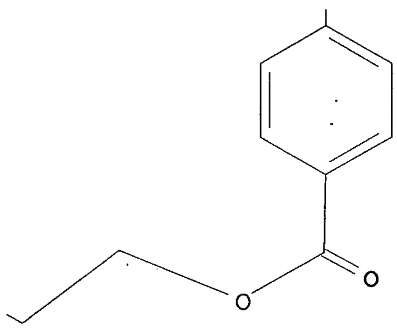


PAGE 3-A



PAGE 3-B



REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 11 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:726528 HCAPLUS
DOCUMENT NUMBER: 139:371731
TITLE: Photophysical Properties of Directly Linked Linear Porphyrin Arrays
AUTHOR(S): Kim, Dongho; Osuka, Atsuhiro
CORPORATE SOURCE: National Creative Research Initiatives Center for Ultrafast Optical Characteristics Control and Department of Chemistry, Yonsei University, Seoul, 120-749, S. Korea
SOURCE: Journal of Physical Chemistry A (2003), 107(42), 8791-8816
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A variety of porphyrin arrays connected by diverse linkers have been envisaged and prepared for the applications in mol. photonics and electronics. From a viewpoint of operational requirements, the porphyrin arrays should have the very regular pigment arrangements which allow a facile light energy or charge flow along the arrays but do not result in the alteration of individual properties of the constituent pigments leading to formation of so-called energy or charge sink. In these respects, the directly coupled (orthogonal and fused) porphyrin arrays

without any linkers are ideal, because the conformational heterogeneity mainly arising from a dihedral angle distribution between the neighboring porphyrin moieties should be minimized. In addition, the electronic effect of the linker can be disregarded in design strategy of **mol.** photonic **devices**, because the linker can also be considered as a transmission element in electronic communication. Considering these features, these types (orthogonal vs fused) of porphyrin arrays would be one of the most suitable synthetic mol. modules for the realization of **mol.** photonic and electronic **devices**. To unveil the functionalities of various porphyrin arrays, starting from the dihedral angle dependence on the photophys. properties of the porphyrin dimers, we have extended our knowledge to longer orthogonal and fused porphyrin arrays. Overall, the regularly arranged porphyrin arrays with ample electronic interactions will be promising in the applications such as mol. wires, sensors, optical nonlinear materials, and so on.

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 22, 26, 73

ST linear porphyrin array zinc complex photophys property

IT Photonics
(mol.; photophys. properties of directly linked linear porphyrin arrays)

IT Electronic energy transfer
Electronic structure
Electronic transition
Excited singlet state
Fluorescence
Fluorescence up-conversion
HOMO (molecular orbital)
LUMO (molecular orbital)
Molecular electronics
Resonance Raman spectra
(photophys. properties of directly linked linear porphyrin arrays)

IT Ladder **polymers**
Porphyrins
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(photophys. properties of directly linked linear porphyrin arrays)

IT UV and visible spectra
(transient; photophys. properties of directly linked linear porphyrin arrays)

IT 220355-87-3 **486445-24-3** **486445-25-4** 486445-26-5
486445-29-8 **622837-62-1** **622837-63-2**
622837-64-3
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(photophys. properties of directly linked linear porphyrin arrays)

IT **486445-24-3**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(photophys. properties of directly linked linear porphyrin arrays)

RN 486445-24-3 HCAPLUS

CN Zinc, [μ-[5,5',15,15'-tetrakis[4-(1,1-dimethyltridecyl)phenyl]-10,10'-diphenyl-2,2':18,18':20,20'-di(21H,23H-porphinato)(4-)-κN21,κN22,κN23,κN24:κN21',κN22',.kappa .N23',κN24']]di- (9CI) (CA INDEX NAME)

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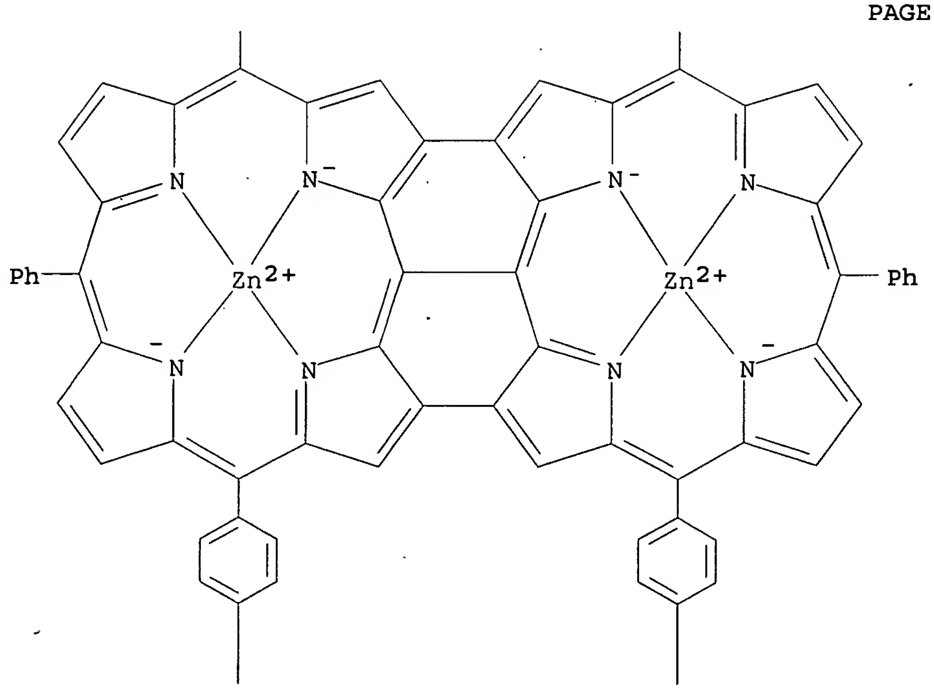

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                    |                                     |
                    Me                                    Me
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REFERENCE COUNT: 121 THERE ARE 121 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 12 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:646098 HCAPLUS
DOCUMENT NUMBER: 139:355420
TITLE: Optical characteristics of PtOEP and Ir(ppy)3 triplet-exciton materials for organic electroluminescence **devices**
AUTHOR(S): Tsuboi, Taiju; Tanigawa, Masayuki
CORPORATE SOURCE: Faculty of Engineering, Kyoto Sangyo University, Kamigamo, Kita-ku, Kyoto, 603-8555, Japan
SOURCE: Thin Solid Films (**2003**), 438-439, 301-307
CODEN: THSFAP; ISSN: 0040-6090
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Absorption and magnetic CD spectra of Pt octaethyl porphine (PtOEP) and tris(2-phenylpyridine) iridium (Ir(ppy)3) films evaporated on fused silica substrate are studied at 13-320 K. The characteristics of absorption bands related with the spin triplet and singlet states are clarified. The energy states of the absorption bands are identified, e.g. relatively weak absorption bands at 485 and 452 nm of Ir(ppy)3 are attributed to the metal-to-ligand charge-transfer spin triplet state (3MLCT). Photoluminescence (PL) and electroluminescence (EL) spectra of PtOEP and Ir(ppy)3 organic EL **devices** with a multi-layer are also investigated, where PtOEP and Ir(ppy)3 mols. are doped in the 4,4'N,N'-dicarbazole-diphenyl host. In the PtOEP EL **device**, an addnl. emission band is observed at 542 nm in the PL and EL spectra, which is due to a hot level of thermally populated triplet state in PtOEP.

CC 73-2 (**Optical**, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 76

ST platinum octaethyl porphine film silica substrate optical absorption spectra; phenyl pyridine iridium film silica substrate optical absorption spectra; photoluminescence electroluminescence platinum octaethyl porphine film light emitting diode; electroluminescence photoluminescence phenyl pyridine iridium film light emitting diode

IT Diodes
(film; optical characteristics of Pt octaethyl porphine and tris(2-phenylpyridine) iridium triplet-exciton materials for organic electroluminescence **devices**)

IT Magnetic circular dichroism
UV and visible spectra
(of Pt octaethyl porphine and tris(2-phenylpyridine) iridium films evaporated on fused silica substrate)

IT Luminescence
Luminescence, electroluminescence
(of organic light-emitting diode **devices** with multilayer films of Pt octaethyl porphine or tris(2-phenylpyridine) iridium)

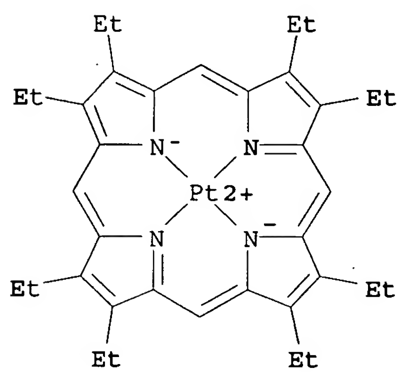
IT **31248-39-2** 94928-86-6, Tris(2-phenylpyridine) iridium

RL: **DEV (Device component use)**; PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
(as film; absorption and magnetic CD spectra of film on fused silica **substrate** and photoluminescence and electroluminescence of organic light-emitting diode with multilayer films)

IT **31248-39-2**
RL: **DEV (Device component use)**; PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
(as film; absorption and magnetic CD spectra of film on fused silica **substrate** and photoluminescence and electroluminescence of organic light-emitting diode with multilayer films)

RN 31248-39-2 HCAPLUS

CN Platinum, [2,3,7,8,12,13,17,18-octaethyl-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

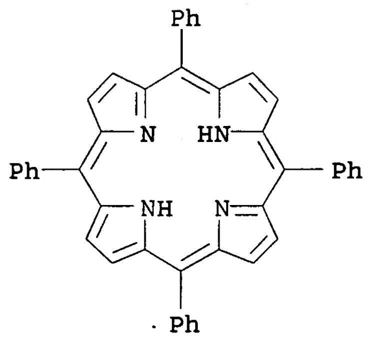
L47 ANSWER 13 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	2003:579201 HCAPLUS
DOCUMENT NUMBER:	139:325889
TITLE:	A double-driven photoelectrochemical cell
AUTHOR(S):	Terasaki, Nao; Kakutani, Keitaro; Akiyama, Tsuyoshi; Yamada, Sunao
CORPORATE SOURCE:	Graduate School of Engineering, Department of Materials Physics and Chemistry, Kyushu University, Higashi-ku, Fukuoka, 812-8581, Japan
SOURCE:	Synthetic Metals **(2003)**, 139(2), 511-514 CODEN: SYMEDZ; ISSN: 0379-6779
PUBLISHER:	Elsevier Science B.V.
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB A novel photoelectrochem. cell consisting of a set of organic thin films which generate photocurrents in opposite directions was fabricated. The poly(3-dodecylthiophene) film containing 5,10,15,20-tetraphenylporphyrin (TPP) and fullerene (C60) generated anodic photocurrents in the presence of ferrocene, while that containing TPP alone generated cathodic photocurrents under aerobic condition. The combination of these two film-modified electrodes showed a better cell performance than the simple sum of these two independent photoelectrochem. cells. A push-pull type, double-driven photoelectrochem. cell is proposed.

CC 52-2 (Electrochemical, Radiational, and Thermal Energy Technology)
Section cross-reference(s): 38, 49, **73**, 76

ST photoelectrochem cell electrode porphyrin fullerene polydodecylthiophene
IR spectra visible
IT Conducting **polymers**
Photocurrent
Photoelectrochemical cells
Photoelectrodes
Photovoltage
(double-driven photoelectrochem. cell with polythiophene-porphyrin-fullerene composite electrodes)
IT Fluoro rubber
Polyimides, uses
Silicone rubber, uses
RL: **DEV (Device component use)**; USES (Uses)
(double-driven photoelectrochem. cell with polythiophene-porphyrin-fullerene composite electrodes)
IT Redox potential
(energy level diagram of; double-driven photoelectrochem. cell with polythiophene-porphyrin-fullerene composite electrodes)
IT Glass, uses
RL: **DEV (Device component use)**; TEM (Technical or engineered material use); USES (Uses)
(**substrate**, ITO-coated; double-driven photoelectrochem. cell with polythiophene-porphyrin-fullerene composite electrodes)
IT 99685-96-8, Fullerene (C60)
RL: **DEV (Device component use)**; USES (Uses)
(C60, composite complexes with PDT and TPP; double-driven photoelectrochem. cell with polythiophene-porphyrin-fullerene composite electrodes)
IT 1273-86-5, Hydroxymethylferrocene
RL: **DEV (Device component use)**; USES (Uses)
(FcOH, electrolyte with NaClO4; double-driven photoelectrochem. cell with polythiophene-porphyrin-fullerene composite electrodes)
IT 104934-53-4, Poly(3-dodecyl thiophene)
RL: **DEV (Device component use)**; PRP (Properties); USES (Uses)
(PDT, composite complexes with TPP and optionally C60; double-driven photoelectrochem. cell with polythiophene-porphyrin-fullerene composite electrodes)
IT **917-23-7P**, 5,10,15,20-Tetraphenylporphyrin
RL: **DEV (Device component use)**; SPN (Synthetic preparation); **PREP (Preparation)**; USES (Uses)
(TPP, composite complexes with PDT and optionally C60; double-driven photoelectrochem. cell with polythiophene-porphyrin-fullerene composite electrodes)
IT 50926-11-9, Indium tin oxide
RL: **DEV (Device component use)**; USES (Uses)
(coated on glass; double-driven photoelectrochem. cell with polythiophene-porphyrin-fullerene composite electrodes)
IT 7601-89-0
RL: **DEV (Device component use)**; USES (Uses)
(electrolyte with FcOH; double-driven photoelectrochem. cell with polythiophene-porphyrin-fullerene composite electrodes)
IT **917-23-7P**, 5,10,15,20-Tetraphenylporphyrin
RL: **DEV (Device component use)**; SPN (Synthetic preparation); **PREP (Preparation)**; USES (Uses)
(TPP, composite complexes with PDT and optionally C60; double-driven photoelectrochem. cell with polythiophene-porphyrin-fullerene composite electrodes)
RN 917-23-7 HCAPLUS
CN 21H,23H-Porphine, 5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 14 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:325832 HCAPLUS
DOCUMENT NUMBER: 139:108298
TITLE: High speed response of organic light emitting diodes and photo-detectors fabricated on a **polymeric substrate** for **polymeric** optical integrated circuits
AUTHOR(S): Ohmori, Yutaka; Kajii, Hirotake; Taneda, Takayuki; Kaneko, Masamitsu; Fujiki, Tsubasa; Takahashi, Kazuya
CORPORATE SOURCE: Collaborative Research Center for Advanced Science and Technology (CRCAST), Osaka University, Osaka, 565-0871, Japan
SOURCE: Materials Research Society Symposium Proceedings (**2002**), 736(Electronics on Unconventional Substrates--Electrotextiles and Giant-Area Flexible Circuits), 233-238
CODEN: MRSPDH; ISSN: 0272-9172
PUBLISHER: Materials Research Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Organic electroluminescent diode (OELD) was studied for use as a light source of **polymeric** optical integrated **devices.** The OLED was fabricated by organic mol. beam deposition (OMBD) technique. The OLEDs were fabricated on both glass and **polymeric substrates.** The **device** fabricated on a **polymeric substrate** shows similar **device** characteristics to those on a glass substrate. Optical signals of faster than 100 MHz was created by applying pulsed voltages directly to the rubrene doped OLED. Optical photo detectors (OPDs) using superlattice structure phthalocyanines provide increased pulse response with input optical signals and the response was faster than 1 MHz.

CC 73-11 (**Optical**, Electron, and Mass Spectroscopy and Other Related Properties)

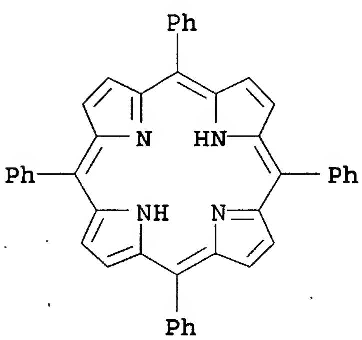
ST electroluminescent **device** photodetector optical integrated circuit phthalocyanine

IT Electroluminescent **devices**
Optical detectors
Optical integrated circuits
Superlattices
(high speed response of organic light emitting diodes and photo-detectors fabricated on a **polymeric substrate** for **polymeric** optical integrated circuits)

IT 517-51-1, Rubrene **917-23-7**, Tetraphenyl porphine 2085-33-8, Aluminum tris(8-hydroxyquinolinato) 4733-39-5, Bathocuproine 26201-32-1 31396-84-6 123847-85-8, α-NPD
RL: **DEV (Device component use)**; PRP (Properties); USES (Uses)
(high speed response of organic light emitting diodes and photo-detectors fabricated on a **polymeric substrate** for **polymeric** optical integrated circuits)

IT **917-23-7**, Tetraphenyl porphine
RL: **DEV (Device component use)**; PRP (Properties); USES (Uses)
(high speed response of organic light emitting diodes and photo-detectors fabricated on a **polymeric substrate** for **polymeric** optical integrated circuits)

RN 917-23-7 HCAPLUS
CN 21H,23H-Porphine, 5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 15 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:247884 HCAPLUS
DOCUMENT NUMBER: 138:398025
TITLE: Covalent Heme Binding to CYP4B1 via Glu310 and a Carbocation Porphyrin Intermediate
AUTHOR(S): Zheng, Yi-Min; Baer, Brian R.; Kneller, M. Byron; Henne, Kirk R.; Kunze, Kent L.; Rettie, Allan E.
CORPORATE SOURCE: Department of Medicinal Chemistry, School of Pharmacy, University of Washington, Seattle, WA, 98195, USA
SOURCE: Biochemistry (**2003**), 42(15), 4601-4606
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Recently we found that CYP4B1, and several other members of the CYP4 family of enzymes, are covalently linked to their prosthetic heme group through an ester linkage. In the current study, we mutated a conserved CYP4 I-helix residue, E310 in rabbit CYP4B1, to glycine, alanine, and aspartate to examine the effect of these mutations on the extent of covalent heme binding and catalysis. All mutants expressed well in insect cells and were isolated as a mixture of monomeric and dimeric forms as determined by LC/ESI-MS of the intact proteins. Rates of metabolism decreased in the order E310 > A310 » G310 > D310, with the A310 and G310 mutants exhibiting alterations in regioselectivity for ω-1 and ω-2 hydroxylation of lauric acid, resp. In marked contrast to the wild-type E310 enzyme, the G310, A310, and D310 mutants did not bind heme

covalently. Uniquely, the acid-dissociable heme obtained from the D310 mutant contained an addnl. 16 amu relative to heme and exhibited the same chromatog. behavior as the monohydroxyheme species released upon base treatment of the covalently linked wild-type enzyme. Expression studies with H218O demonstrated incorporation of the heavy isotope from the media into the monohydroxyheme isolated from the D310 mutant at a molar ratio of .apprx.0.8:1. These data show (i) that E310 serves as the site of covalent attachment of heme to the protein backbone of rabbit CYP4B1; (ii) this I-helix glutamate residue influences substrate orientation in the active site of CYP4B1; and (iii) the mechanism of covalent heme attachment most likely involves a carbocation species located on the porphyrin.

CC 7-3 (Enzymes)

ST heme cytochrome CYP4B1 glutamic acid hydroxylation active site

IT Regiochemistry
(Glu310 residue of rabbit cytochrome CYP4B1 binds covalently heme binding and promotes orientation of substrate in active site for catalysis)

IT Carbocations
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(covalent heme binding to CYP4B1 via Glu310 and carbocation porphyrin intermediate)

IT Hydroxylation
(enzymic; Glu310 residue of rabbit cytochrome CYP4B1 binds covalently heme binding and promotes orientation of substrate in active site for catalysis)

IT 56-86-0, L-Glutamic acid, biological studies 143-07-7, Lauric acid, biological studies **14875-96-8**, Heme
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(Glu310 residue of rabbit cytochrome CYP4B1 binds **covalently** heme binding and promotes orientation of **substrate** in active site for catalysis)

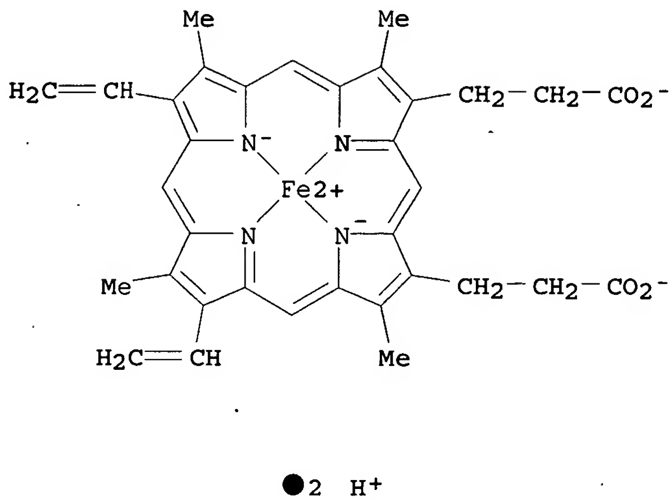
IT 330207-52-8, Cytochrome CYP4B1
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(Glu310 residue of rabbit cytochrome CYP4B1 binds covalently heme binding and promotes orientation of substrate in active site for catalysis)

IT 101-60-0, Porphyrin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(covalent heme binding to CYP4B1 via Glu310 and carbocation porphyrin intermediate)

IT **14875-96-8**, Heme
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(Glu310 residue of rabbit cytochrome CYP4B1 binds **covalently** heme binding and promotes orientation of **substrate** in active site for catalysis)

RN 14875-96-8 HCAPLUS

CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-κN21,κN22,κN23,κN24]-, dihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 16 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:931941 HCAPLUS
DOCUMENT NUMBER: 138:127470
TITLE: Supramolecular Monolayers of Zinc Porphyrin Trimers on Graphite
AUTHOR(S): Yin, J.; Guo, Q.; Palmer, R. E.; Bampos, N.; Sanders, J. K. M.
CORPORATE SOURCE: Nanoscale Physics Research Laboratory, School of Physics and Astronomy, University of Birmingham, Edgbaston /Birmingham, B15 2TT, UK
SOURCE: Journal of Physical Chemistry B (**2003**), 107(1), 209-216
CODEN: JPCBFK; ISSN: 1520-6106
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

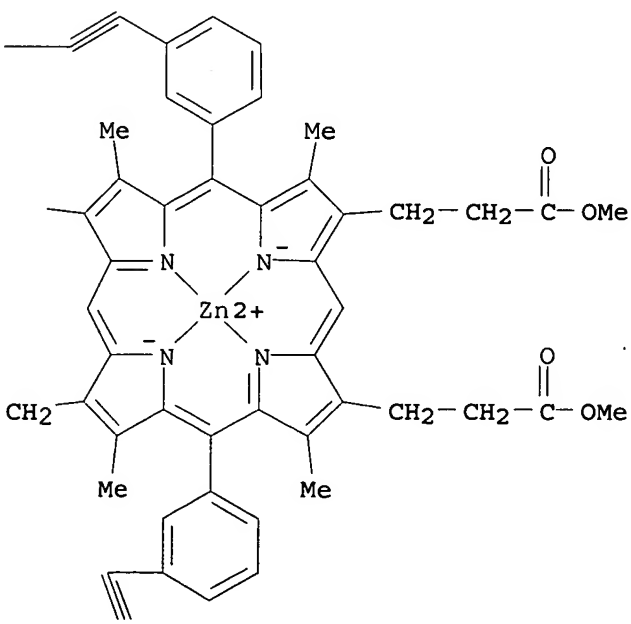
AB Zinc porphyrin trimers have been deposited on highly oriented pyrolytic graphite (HOPG) from the liquid phase. By controlling the concentration of the solution and deposition parameters, we have prepared single mol. layers. The mol. monolayers, as characterized using both atomic force microscopy (AFM) and scanning tunneling microscopy (STM), are amorphous. The trimer mols. adopt a uniform adsorption orientation with the component porphyrin rings perpendicular to the substrate, giving rise to a monolayer film thickness of 1.7 ± 0.2 nm, which is characteristic of the height of the individual mols. STM imaging of the mol. layers was conducted both in vacuum and in air, giving identical results. This type of mol. monolayer provides a useful platform for the study of surface and interface phenomena outside a vacuum system and is potentially useful for practical fabrication of **mol. devices** because of the simplicity of the sample preparation and the stability of the interface in ambient.

CC 66-3 (Surface Chemistry and Colloids)
ST supramol monolayer zinc porphyrin trimer graphite
IT Surface structure
(STM and AFM images; supramol. monolayer of zinc porphyrin trimer on graphite studied using)
IT Monolayers

    (supramol. monolayer of zinc porphyrin trimer on graphite)
IT Thickness
    (supramol. monolayer of zinc porphyrin trimer on graphite studied using)
IT 7782-42-5, Graphite, uses
    RL: NUU (Other use, unclassified); USES (Uses)
    (supramol. monolayer of zinc porphyrin trimer on graphite)
IT **130829-47-9**
    RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
    (supramol. monolayer of zinc porphyrin trimer on graphite)
IT **130829-47-9**
    RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
    (supramol. monolayer of zinc porphyrin trimer on graphite)
RN 130829-47-9 HCAPLUS
CN Zinc, [μ3-[dodecamethyl 18,24,43,49,68,74,77,83,92,98,105,111-dodecamethyl-85,86,87,88,100,101,113,114,117,118,119,120-dodecaazadocosacyclo[64.9.9.916,26.941,51.12,6.111,15.117,20.122,25.127,31.136,40.142,45.147,50.152,56.161,65.167,70.172,75.176,79.181,84.191,94.196,99.1104,107.1109,112]eicosahectahenpentacontaene-7,9,32,34,57,59-hexayne-19,23,44,48,69,73,78,82,93,97,106,110-dodecapropanoato(6-)-κN85,κN86,κN87,κN88:κN100,κN101,.kappa.N119,κN120:κN113,κN114,κN117,κN118]]tri-
    (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

PAGE 1-B



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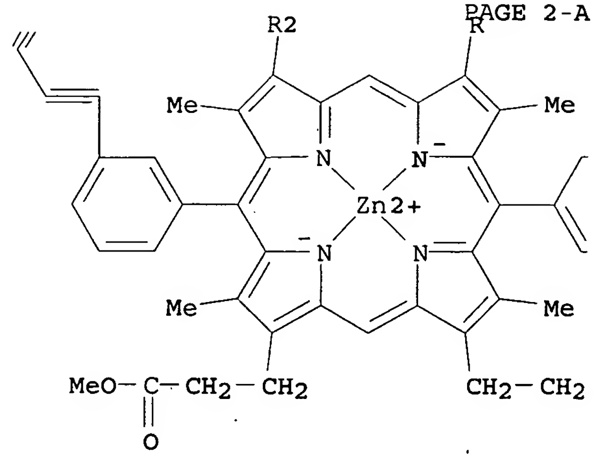

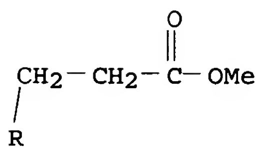

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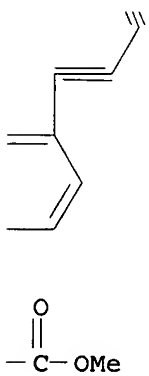

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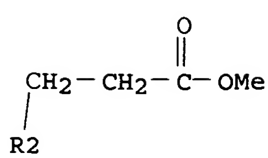


REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 17 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:536617 HCAPLUS
DOCUMENT NUMBER: 137:239568
TITLE: Charge transport in photofunctional nanoparticles self-assembled from zinc 5,10,15,20-tetrakis(perylene-diimide)porphyrin building blocks
AUTHOR(S): van der Boom, Tamar; Hayes, Ryan T.; Zhao, Yongyu; Bushard, Patrick J.; Weiss, Emily A.; Wasielewski, Michael R.
CORPORATE SOURCE: Center for Nanofabrication and Molecular Self-Assembly, Department of Chemistry, Northwestern University, Evanston, IL, 60208-3113, USA
SOURCE: Journal of the American Chemical Society (**2002**), 124(32), 9582-9590
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Mols. designed to carry out photochem. energy conversion typically employ several sequential electron transfers, as do photosynthetic proteins. Yet, these mols. typically do not achieve the extensive charge-transport characteristic of semiconductor **devices.** The authors have prepared a large mol. in which four perylene-3,4:9,10-tetracarboxydiimide (PDI) units that both collect photons and accept electrons are attached to a central zinc 5,10,15,20-tetraphenylporphyrin (ZnTPP) electron donor. This mol. self-assembles into ordered nanoparticles both in solution and in the solid-state, driven by van der Waals stacking of the PDI mols. Photoexcitation of the nanoparticles results in quant. charge separation in 3.2 ps to form ZnTPP+PDI- radical ion pairs, in which the radical anion rapidly migrates to PDI mols. that are, on average, 21 Å away, as evidenced by magnetic field effects on the yield of the PDI triplet state that results from radical ion pair recombination. These nanoparticles exhibit charge transport properties that combine important features from both photosynthetic and semiconductor photoconversion systems. A supporting information regarding synthesis and characterization of the mols. used as well as kinetic simulations are available at http://pubs.acs.organic

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 72, **73**

ST photofunctional nanoparticle selfassembled zinc perylenediimide porphyrin photoinduced charge transfer; electron transport photofunctional nanoparticle selfassembled zinc perylenediimide porphyrin

IT Photosystems
(antenna complex; charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin in relation to)

IT Electron transport
Nanoparticles
Self-assembly
Van der Waals force
(charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin building blocks)

IT Oscillator strength
(charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin on quartz **substrate**)

IT Electron transfer
Electron transfer
(intramol., photochem.; charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin building blocks)

IT Radical ions
(pairs, intramol.; photoinduced intramol. electron transfer in self-assembled zinc tetrakis(perylene-diimide)porphyrin and intersystem crossing of photoproduced radical ion pair)

IT Free energy
(photoinduced intramol. electron transfer in nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin building blocks)

IT Excited triplet state
Intersystem crossing
Magnetic field effects
Zeeman effect
(photoinduced intramol. electron transfer in self-assembled zinc tetrakis(perylene-diimide)porphyrin and intersystem crossing of photoproduced radical ion pair)

IT Electrochemistry
(spectroelectrochem.; charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin on quartz **substrate**)

IT Optical absorption
(transient; charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin building blocks)

IT 1923-70-2, Tetra-n-Butylammonium perchlorate
RL: NUU (Other use, unclassified); USES (Uses)
(electrolyte; electrochem. study of charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin)

IT 457916-29-9P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(ion-pair photoproduct; charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin building blocks)

IT 1138-52-9, 3,5-Di-tert-butylphenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with 1,7-Dibromoperylene-3,4:9,10-tetracarboxydianhydride)

IT 118129-60-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with 3,5-di-tert-butylphenol)

IT 404871-21-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction with ethylhexylamine)

IT 457892-77-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction with tetrakis(p-aminophenyl)porphyrin)

IT 457915-36-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction with zinc acetate)

IT 457892-79-4P **457892-80-7P**
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(reference compound; charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin building blocks)

IT **457892-78-3P**

RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(reference ion-pair photoproduct; charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin building blocks)

IT 81-33-4
RL: PRP (Properties)
(reference; charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin building blocks)

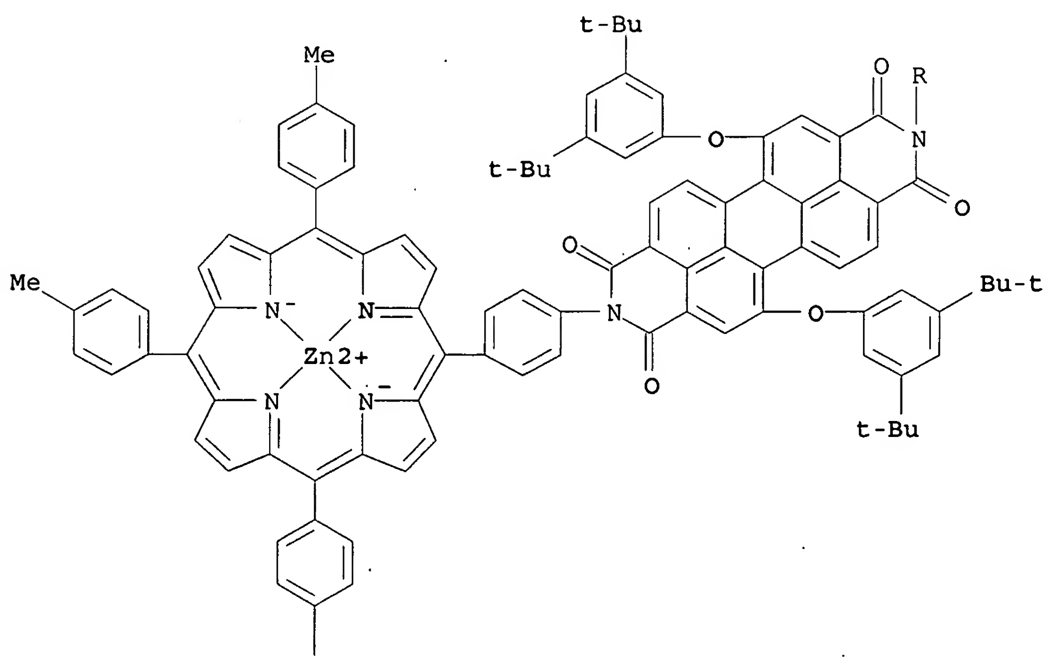
IT 60676-86-0, Vitreous silica
RL: NUU (Other use, unclassified); USES (Uses)
(**substrate**; charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin on quartz **substrate**)

IT **457892-80-7P**
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(reference compound; charge transport in photofunctional nanoparticles self-assembled from zinc tetrakis(perylene-diimide)porphyrin building blocks)

RN 457892-80-7 HCAPLUS

CN Zinc, [2-[5-[5,12-bis[3,5-bis(1,1-dimethylethyl)phenoxy]-9-(2-ethylhexyl)-3,8,9,10-tetrahydro-1,3,8,10-tetraoxoanthra[2,1,9-def:6,5,10-d'e'f']diisoquinolin-2(1H)-yl]-2,7-bis(1,1-dimethylethyl)-9,9-dimethyl-9H-xanthen-4-yl]-5,12-bis[3,5-bis(1,1-dimethylethyl)phenoxy]-9-[4-[10,15,20-tris(4-methylphenyl)-21H,23H-porphin-5-yl-κN21,κN22,κN23,κN24]phenyl]anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetronato(2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

PAGE 1-A



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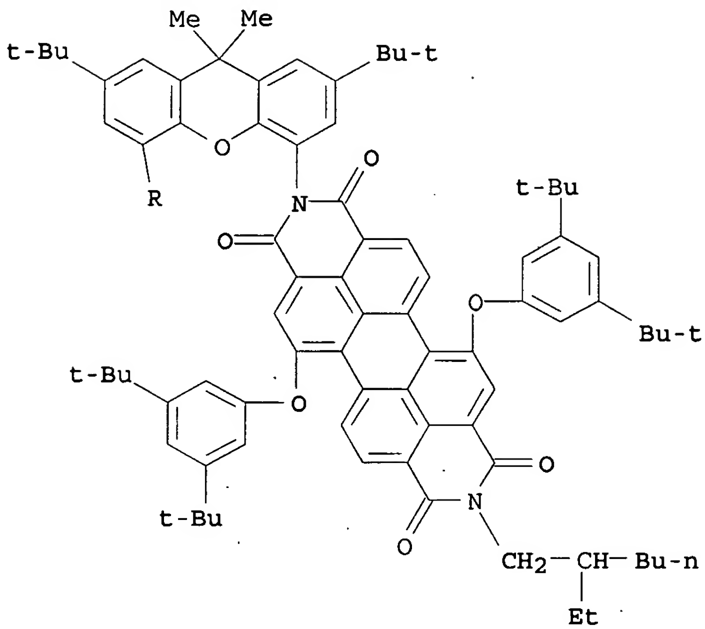
PAGE 3-A



REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 18 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:533846 HCAPLUS
DOCUMENT NUMBER: 137:285561
TITLE: Potential modulation reflectance of manganese halogenated tetraphenylporphyrin derivatives assembled on gold electrodes
AUTHOR(S): Yamada, Taku; Nango, Mamoru; Ohtsuka, Toshiaki
CORPORATE SOURCE: Graduate School of Engineering, Division of Molecular Chemistry, Hokkaido University, Sapporo, 060-8628, Japan
SOURCE: Journal of Electroanalytical Chemistry (**2002**), 528(1-2), 93-102
CODEN: JECHES
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Electron transfer from/to redox manganese porphyrin self-assembled monolayers (SAMs) on gold electrodes in DMSO solution was studied by potential-modulation reflectance, i.e. electroreflectance (ER) with cyclic voltammetry and a.c. impedance. The ER voltammogram reveals more clearly the redox waves of Mn(III)/Mn(II) in the porphyrin monolayers than the cyclic voltammogram (CV). The standard rate consts. of electron transfer, i.e. turn-over number of the redox reaction at the formal potential was

evaluated from complex plane plots of ER of the manganese redox couples. On the complex plane plot of the ER, the rate constant can be determined from a characteristic frequency of the a.c. response. The rate consts. thus obtained were compared with the values evaluated from the impedance data and further compared with the values calculated by Sagara's treatment from the relation between the phase retardation and the frequency of the complex ER data. Fairly good agreement was obtained between the rate consts. from the three evaluations. The ER response is comparable to the complex capacitance defined as (dQ/dE) for the circuit involving the redox couple. The rate consts. increase with a decrease in a distance between the electrode **substrate** and the redox manganese porphyrin and depend on the species bound to Ph groups around the porphyrin unit in the order of Cl > H > F.

CC 72-2 (Electrochemistry)
Section cross-reference(s): 66, 67, **73**, 78

ST potential modulation reflectance manganese halogenated tetraphenylporphyrin deriv assembled gold; kinetics electron exchange manganese halogenated thioalkyl tetraphenylporphyrin deriv

IT Electrooptical effect
(UV-visible electroreflection spectra; of manganese thioalkyl halogenated phenylporphyrin derivative monolayers assembled on gold electrodes in DMSO)

IT Reflection spectra
(UV-visible electroreflection; of manganese thioalkyl halogenated phenylporphyrin derivative monolayers assembled on gold electrodes in DMSO)

IT Redox reaction
(electrochem.; of manganese thioalkyl halogenated phenylporphyrin derivative monolayers assembled on gold electrodes)

IT UV and visible spectra
(electroreflection; of manganese thioalkyl halogenated phenylporphyrin derivative monolayers assembled on gold electrodes in DMSO)

IT Chemical chains
(length, alkyl; of thioalkylhalophenylporphyrin manganese complex in electron transfer kinetics of monolayer on gold)

IT Electric capacitance
(of manganese thioalkyl halogenated phenylporphyrin derivative monolayers assembled on gold electrodes)

IT Cyclic voltammetry
Electric impedance
Electron transfer
Electron transfer
(of manganese thioalkyl halogenated phenylporphyrin derivative monolayers assembled on gold electrodes in DMSO)

IT UV and visible spectra
(of manganese thioalkyl halogenated phenylporphyrin derivative monolayers assembled on gold electrodes in DMSO and in aqueous Na2S2O4)

IT Equivalent electric circuits
(of manganese thioalkylhalophenylporphyrin complex monolayer on gold electrode)

IT Substituent effects
(on electron transfer kinetics of manganese complexes with thioalkylhalophenylporphyrin)

IT Self-assembled monolayers
(potential modulation reflectance of manganese halogenated thioalkyl phenylporphyrin derivs. assembled monolayers on gold electrodes)

IT 7775-14-6, Sodium dithionite
RL: NUU (Other use, unclassified); PRP (Properties); USES (Uses)
(absorption spectra of manganese halogenated thioalkyl phenylporphyrin derivs. monolayers on gold electrodes in aqueous)

IT 7440-57-5, Gold, uses

RL: CPS (Chemical process); DEV (Device component use); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process); USES (Uses)
(electron transfer kinetics and potential modulation reflectance of manganese thioalkyl halogenated phenylporphyrin derivative monolayers assembled on gold electrodes in DMSO)

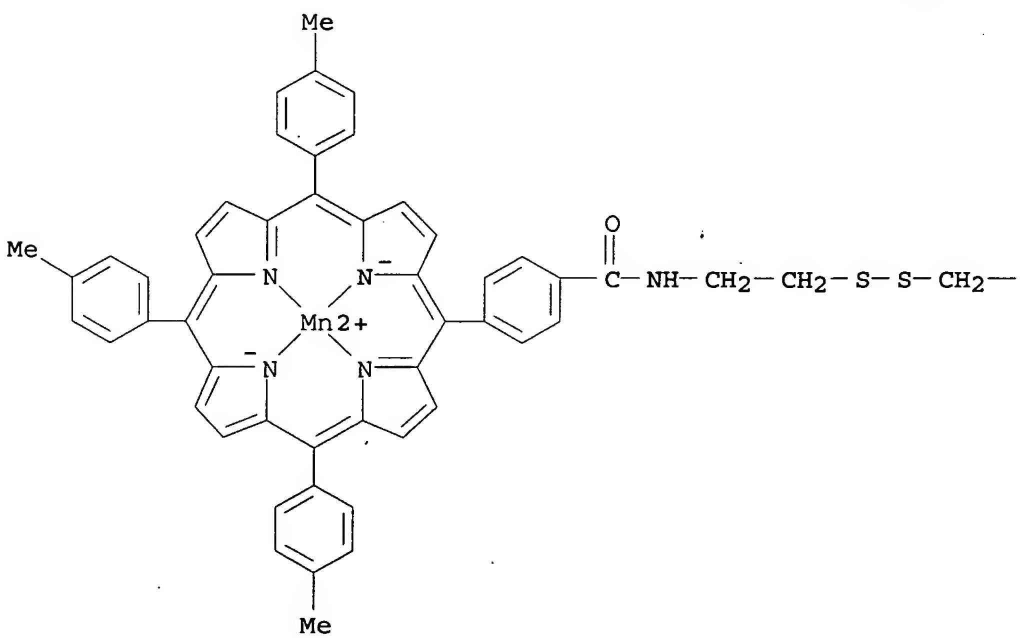
IT **203567-69-5 203567-74-2 203567-95-7**
204441-73-6 357417-94-8 357417-95-9
357417-96-0 357417-97-1 357417-98-2
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(electron transfer kinetics and potential modulation reflectance of manganese thioalkyl halogenated phenylporphyrin derivative monolayers assembled on gold electrodes in DMSO)

IT **203567-69-5**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(electron transfer kinetics and potential modulation reflectance of manganese thioalkyl halogenated phenylporphyrin derivative monolayers assembled on gold electrodes in DMSO)

RN 203567-69-5 HCAPLUS

CN Manganese, [μ-[[N,N'-(dithiodi-2,1-ethanediyl)bis[4-[10,15,20-tris(4-methylphenyl)-21H,23H-porphin-5-yl-κN21,κN22,κN23,.kappa .N24]benzamidato]](4-)]]di- (9CI) (CA INDEX NAME)

PAGE 1-A



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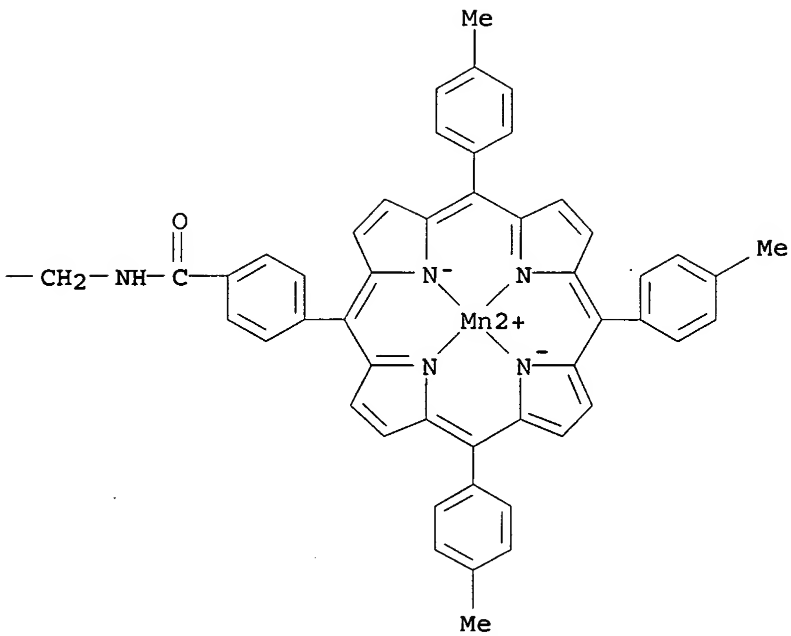


REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 19 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	2002:450171 HCAPLUS
DOCUMENT NUMBER:	137:40483
TITLE:	Molecular architecture for molecular electro-optical transistor and switch
INVENTOR(S):	Simic-Glavaski, Branimir
PATENT ASSIGNEE(S):	USA
SOURCE:	U.S. Pat. Appl. Publ., 26 pp. CODEN: USXXCO
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002071168	A1	20020613	US 2001-14659	20011211 <--
US 6937379	B2	20050830		
WO 2002049124	A2	20020620	WO 2001-US47638	20011211 <--
WO 2002049124	A3	20030130		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AU 2002028957	A5	20020624	AU 2002-28957	20011211 <--

EP 1344219 A2 20030917 EP 2001-990084 20011211 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2004536714 T2 20041209 JP 2002-550328 20011211 <--
US 2006001943 A1 20060105 US 2005-214333 20050829 <--
PRIORITY APPLN. INFO.: US 2000-254667P P 20001211 <--
US 2001-14659 A1 20011211 <--
WO 2001-US47638 W 20011211 <--

AB Switching **devices** and memory **devices** are described which comprise a macrocyclic mol. arrangement in ≥1 of a substantially one-dimensional stack arrangement or a two-dimensional arrangement, the arrangement being adsorbed on a substrate. Reversible quantum switches with multiple outputs comprising the switching **devices** and information storage and retrieval apparatus comprising the memory **devices** are also described, as are methods of obtaining multiple outputs from the switching **devices.** In operation, response to a stimulus may be detected using Raman spectrometry, NMR, or tunneling microscopy techniques. More specifically, **mol** ./quantum **devices** are described which comprise a monomeric metalated phthalocyanine that behaves as a fast (<10-12 s) energy efficient (30 kT/bit of information) fully reversible quantum switch with multiple outputs. Methods of making a **mol.**/quantum **device** comprising a monomeric metalated phthalocyanine that behaves as a fast, energy efficient fully reversible quantum switch with multiple outputs wherein the monomeric phthalocyanines are organized in structural combinations of ≥1 of one-dimensional wire-like ring-stacked or two-dimensional sheet-like ring-fused phthalocyanines are described which entail tailoring the number of peaks in a cyclic voltammogram representation of operation of the **device** according to the number of stacked rings in the wire. Method of making a quantum electro-optical **device**, comprising arranging a plurality of macrocyclic mols. in a substantially one-dimensional ring-like stack or in a substantially two-dimensional sheet-like arrangement, and adsorbing the same on a conductor or semiconductor substrate.

IC ICM G02F001-03
ICS G02F001-07

INCL 359253000; X35-925.2

CC 76-14 (Electric Phenomena)
Section cross-reference(s): **73**

ST switching **device** adsorbed macrocyclic **mol** stack; memory **device** adsorbed macrocyclic **mol** stack; quantum **device** adsorbed macrocyclic **mol** stack

IT NMR (nuclear magnetic resonance)
Raman spectroscopy
(in operation of switching and memory **devices** based on macrocyclic **mol.** stacks adsorbed on substrates)

IT Adsorbed substances
Electrooptical switches
Memory **devices**
Molecular electronic **devices**
Quantum **devices**
Transistors
(switching and memory **devices** based on macrocyclic **mol.** stacks adsorbed on substrates and their production and use and operation)

IT Chlorophylls, processes
Cytochromes
Porphyrins
RL: **DEV (Device component use)**; PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)

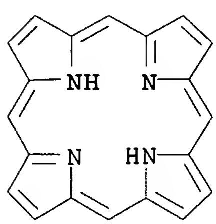
(switching and memory **devices** based on macrocyclic **mol.** stacks adsorbed on substrates and their production and use and operation)

IT Electron microscopy
(tunneling; in operation of switching and memory **devices** based on macrocyclic **mol.** stacks adsorbed on substrates)

IT **101-60-0**, Porphyrin 132-16-1, Iron phthalocyanine 1277-38-9 7429-90-5D, Aluminum, compds. with macrocyclic mols. 7439-89-6D, Iron, compds. with macrocyclic mols. 7440-02-0D, Nickel, compds. with macrocyclic mols. 7440-05-3D, Palladium, compds. with macrocyclic mols. 7440-06-4D, Platinum, compds. with macrocyclic mols. 7440-22-4, Silver, processes 7440-22-4D, Silver, compds. with macrocyclic mols. 7440-48-4D, Cobalt, compds. with macrocyclic mols. 7440-50-8D, Copper, compds. with macrocyclic mols. 7440-57-5D, Gold, compds. with macrocyclic mols. **14875-96-8**, Heme 19333-15-4D, compds. 33308-41-7
RL: **DEV (Device component use)**; PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(switching and memory **devices** based on macrocyclic **mol.** stacks adsorbed on **substrates** and their production and use and operation)

IT **101-60-0**, Porphyrin
RL: **DEV (Device component use)**; PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(switching and memory **devices** based on macrocyclic **mol.** stacks adsorbed on **substrates** and their production and use and operation)

RN 101-60-0 HCAPLUS
CN 21H,23H-Porphine (9CI) (CA INDEX NAME)



REFERENCE COUNT: 83 THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 20 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:365333 HCAPLUS
DOCUMENT NUMBER: 137:102969
TITLE: Structural, Spectroscopic, and Reactivity Comparison of Xanthene- and Dibenzofuran-Bridged Cofacial Bisporphyrins
AUTHOR(S): Chang, Christopher J.; Baker, Erin A.; Pistorio, Bradford J.; Deng, Yongqi; Loh, Zhi-Heng; Miller, Scott E.; Carpenter, Scott D.; Nocera, Daniel G.
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SOURCE: Inorganic Chemistry (**2002**), 41(12), 3102-3109
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:102969

AB A comparison of the structure, spectroscopy, and oxygen atom-transfer reactivity of cofacial bisporphyrins anchored by xanthene (DPX) and dibenzofuran (DPD) pillars is presented. The synthesis and characterization of dicopper(II) and dinickel(II) complexes of DPD completes a homologous series of homobimetallic zinc(II), copper(II), and nickel(II) complexes for both cofacial platforms. X-ray crystallog. anal. of the parent free-base porphyrins H4DPX (1) and H4DPD (5) confirms the face-to-face arrangement of the two porphyrin macrocycles with a large available range of vertical pocket sizes: 1 (C80H92Cl2N8O), triclinic, space group P.hivin.1, a 13.5167(12), b 21.7008(18), c 23.808(2) Å, α 80.116(2), β 76.832(2), γ 80.4070(10)°, Z = 4; 5 (C80H83N8O2), monoclinic, space group C2/c, a 22.666(2), b 13.6749(14), c 42.084(4) Å, β 94.554(2)°, Z = 8. EPR spectroscopy of dicopper(II) derivs. Cu2DPX (3) and Cu2DPD (7) complements the crystallog. studies by probing intramol. metal-metal arrangements in frozen solution Exciton interactions between the porphyrin subunits in fluid solution are revealed by steady-state and time-resolved electronic absorption and emission spectroscopy. The resulting compilation of structural and spectroscopic data provides a benchmark for the use of these and related platforms for the activation of small-mol. **substrates.** A structure-function relation is developed for the photoinduced oxygen atom-transfer reactions of bisiron(III) μ-oxo derivs. of DPX and DPD. The efficiency of the photochem. process is markedly dependent (.apprx.104-fold) on the vertical flexibility of cofacial architecture provided by the spacer.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 26, 73, 74, 75

ST transition metal xanthene dibenzofuran bridged cofacial porphyrin structure photochem; crystal structure xanthene dibenzofuran bridged cofacial porphyrin; iron xanthene dibenzofuran bridged cofacial porphyrin prepn photochem reactivity; phosphite reaction iron xanthene dibenzofuran bridged cofacial porphyrin complex; fluorescence xanthene dibenzofuran bridged cofacial porphyrin zinc complex

IT Homologous series
(crystallog. derived geometrical features, UV-visible spectra and fluorescence of homologous series of transition metal xanthene- and dibenzofuran-bridged cofacial bisporphyrin complexes)

IT Crystal structure
(of xanthene- and dibenzofuran-bridged cofacial bisporphyrins)

IT Molecular structure
(of xanthene- and dibenzofuran-bridged cofacial bisporphyrins and their homobimetallic transition metal complexes)

IT Fluorescence
(of xanthene- and dibenzofuran-bridged cofacial bisporphyrins and their zinc complexes)

IT Substitution reaction, coordinative
(photochem., reductive; photoinduced oxygen atom-transfer reactions of phosphites with iron xanthene-/dibenzofuran-bridged cofacial bisporphyrin oxo dinuclear complexes)

IT Transition metal complexes
RL: PRP (Properties)
(porphyrin; crystallog. derived geometrical features, UV-visible spectra and fluorescence of homologous series of homobimetallic transition metal xanthene- and dibenzofuran-bridged cofacial bisporphyrin complexes)

IT Metalloporphyrins
RL: PRP (Properties)
(transition metal; crystallog. derived geometrical features, UV-visible

spectra and fluorescence of homologous series of homobimetallic transition metal xanthene- and dibenzofuran-bridged cofacial bisporphyrin complexes)

IT **259669-11-9 261724-78-1**
RL: PRP (Properties)
(crystallog. derived geometrical features, UV-visible spectrum and fluorescence in homologous series in comparison of xanthene- and dibenzofuran-bridged analogs)

IT **261724-79-2 261724-80-5**
RL: PRP (Properties)
(crystallog. derived geometrical features, UV-visible spectrum in homologous series in comparison of xanthene- and dibenzofuran-bridged analogs)

IT **259669-12-0**
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(crystallog. derived geometrical features, and photoinduced oxygen atom-transfer reactions with phosphites in comparison of xanthene- and dibenzofuran-bridged analogs)

IT 116-17-6, Triisopropylphosphite 1795-31-9, Tris(trimethylsilyl)phosphite
RL: RCT (Reactant); RACT (Reactant or reagent)
(photoinduced oxygen atom-transfer reactions with iron xanthene-/dibenzofuran-bridged cofacial bisporphyrin oxo dinuclear complexes)

IT **442197-51-5P 442197-52-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and UV-visible spectrum in homologous series in comparison of xanthene- and dibenzofuran-bridged analogs)

IT **442197-53-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photoinduced oxygen atom-transfer reactions with phosphites in comparison of xanthene- and dibenzofuran-bridged analogs)

IT **442197-54-8P 442197-55-9P 442197-56-0P**
442197-57-1P 442197-58-2P 442197-59-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation from photoinduced oxygen atom-transfer reaction of phosphite with iron xanthene-/dibenzofuran-bridged cofacial bisporphyrin oxo dinuclear complex)

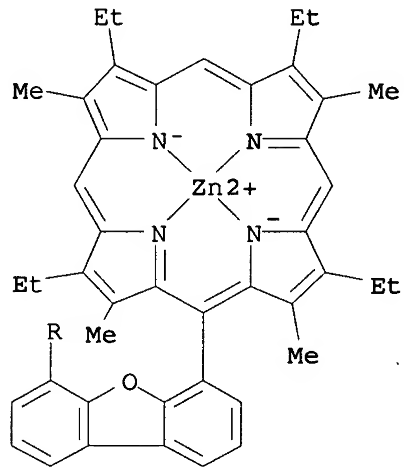
IT 259669-10-8P 261724-77-0P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, crystal and mol. structure, UV-visible spectrum and fluorescence in homologous series in comparison of xanthene- and dibenzofuran-bridged analogs, and complexation with transition metals)

IT **259669-11-9**
RL: PRP (Properties)
(crystallog. derived geometrical features, UV-visible spectrum and fluorescence in homologous series in comparison of xanthene- and dibenzofuran-bridged analogs)

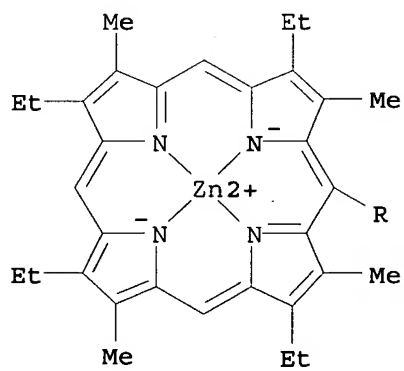
RN 259669-11-9 HCAPLUS

CN Zinc, [μ-[[5,5'-(4,6-dibenzofurandiyl)bis[2,8,13,17-tetraethyl-3,7,12,18-tetramethyl-21H,23H-porphinato-κN21,κN22,κN23,κN24]](4-)]]di- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 21 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:357890 HCAPLUS
DOCUMENT NUMBER: 137:87484
TITLE: Supramolecular Fullerene-Porphyrin Chemistry. Fullerene Complexation by Metalated "Jaws Porphyrin" Hosts
AUTHOR(S): Sun, Dayong; Tham, Fook S.; Reed, Christopher A.; Chaker, Leila; Boyd, Peter D. W.
CORPORATE SOURCE: Departments of Chemistry, University of California, Riverside, 92521-0403, USA
SOURCE: Journal of the American Chemical Society (**2002**), 124(23), 6604-6612
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:87484

AB Porphyrins and fullerenes are spontaneously attracted to each other. This new supramol. recognition element is explored in discrete, soluble, coordinatively linked porphyrin and metalloporphyrin dimers. Jawlike clefts in these bis-porphyrins are effective hosts for fullerene guests. X-ray structures of the Cu complex with C60 and free-base complexes with C70 and a pyrrolidine-derivatized C60 were obtained. The electron-rich 6:6 ring-juncture bonds of C60 show unusually close approach to the porphyrin or metalloporphyrin plane. Binding consts. in toluene solution increase in the order Fe(II) < Pd(II) < Zn(II) < Mn(II) < Co(II) < Cu(II) < 2H and span the range 490-5200 M-1. Unexpectedly, the free-base porphyrin binds C60 more strongly than the metalated porphyrins. This is ascribed to electrostatic forces, enhancing the largely van der Waals forces of the π-π interaction. The ordering with metals is ascribed to a subtle interplay of solvation and weak interaction forces. Conflicting opinions on the relative importance of van der Waals forces, charge transfer, electrostatic attraction, and coordinate bonding are addressed. The supramol. design principles arising from these studies have potential applications in the preparation of photophys. **devices**, **mol.** magnets, **mol.** conductors, and porous metal-organic frameworks.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 65, 68, 75

ST fullerene inclusion binding transition metal porphyrin; crystal structure copper palladium porphyrin fullerene inclusion

IT Formation constant
(binding consts. of bis-porphyrin host guest complexes with fullerenes)

IT Binding energy
Crystal structure
Molecular structure
Pi-pi interaction
(of bis-porphyrin host guest complexes with fullerenes)

IT Transition metal complexes
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(porphyrin; preparation of bis-porphyrin host guest complexes with fullerenes)

IT Inclusion reaction
(preparation of bis-porphyrin host guest complexes with fullerenes)

IT Fullerenes
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(preparation of bis-porphyrin host guest complexes with fullerenes)

IT Porphyrins
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bis-porphyrin host guest complexes with fullerenes)

IT Inclusion compounds
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal structure, binding interactions and binding energy of bis-porphyrin host guest complexes with fullerenes)

IT Metalloporphyrins
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(transition metal; preparation of bis-porphyrin host guest complexes with fullerenes)

IT 440089-39-4
RL: PRP (Properties)
(host guest binding energy and optimized mol. structure)

IT 99685-96-8, C60 Fullerene
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)

(host guest complexation and binding energy and binding consts. with bis-porphyrins)

IT 135113-16-5, Fullerene-C84 142979-02-0, Gadolinium fulleride (GdC82)
RL: RCT (Reactant); RACT (Reactant or reagent)
(host guest complexation with bis-porphyrin)

IT 115383-22-7, C70 Fullerene
RL: RCT (Reactant); RACT (Reactant or reagent)
(host guest complexation with bis-porphyrins)

IT 151872-44-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(host guest complexation with fullerene)

IT **440089-35-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(host guest complexation with fullerenes and binding energy and binding constant with C60)

IT 440089-28-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and binding energy with C60 fullerene)

IT **440089-36-1P 440089-37-2P 440356-12-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure)

IT **312327-69-8P 440356-14-9P 440356-17-2P 440356-18-3P 440356-24-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and host guest binding constant)

IT **440089-42-9P 440356-13-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 440089-40-7P **440089-41-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation, host guest binding energy and optimized mol. structure)

IT **312327-68-7P 440089-30-5P 440089-31-6P 440089-32-7P 440089-33-8P 440089-34-9P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, host guest complexation with fullerenes and binding constant with C60)

IT 440089-29-2P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, host guest complexation with fullerenes and binding energy with C60)

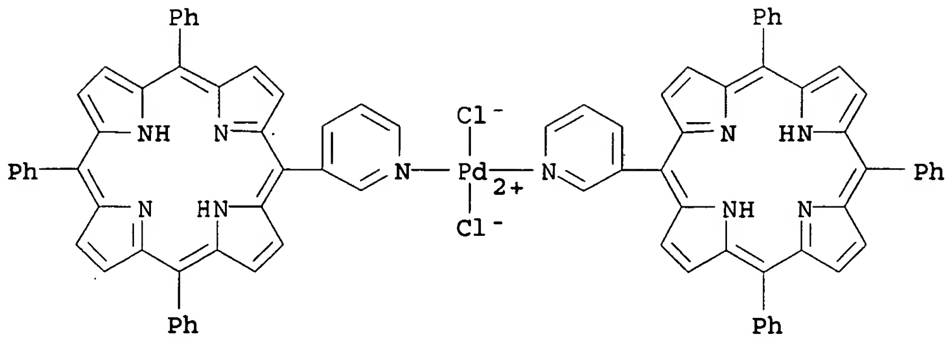
IT **440356-16-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation, mol. structure and host guest binding constant)

IT 99-63-8, 1,3-Di(chlorocarbonyl)benzene 100-20-9, 1,4-Di(chlorocarbonyl)benzene 12386-08-2, Bis(DMSO)dichloropalladium 78265-41-5 79123-22-1, meso-Triphenyl(3-pyridyl)porphyrin
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of bis-porphyrin for host guest complexation with fullerenes)

IT **440089-35-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(host guest complexation with fullerenes and binding energy and binding constant with C60)

RN 440089-35-0 HCAPLUS

CN Palladium, dichlorobis[5,10,15-triphenyl-20-(3-pyridinyl-κN)-21H,23H-porphine]-, (SP-4-1)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 22 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:340182 HCAPLUS
DOCUMENT NUMBER: 137:69900

TITLE: Weakly Coupled Molecular Photonic Wires: Synthesis and Excited-State Energy-Transfer Dynamics

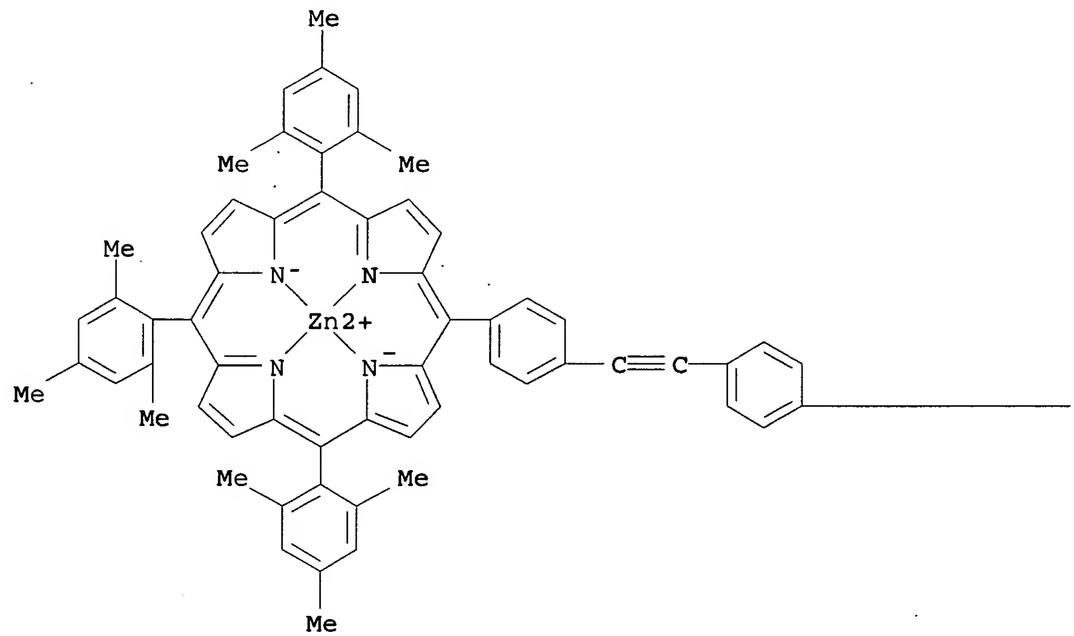
AUTHOR(S): Ambroise, Arounaguiry; Kirmaier, Christine; Wagner, Richard W.; Loewe, Robert S.; Bocian, David F.; Holten, Dewey; Lindsey, Jonathan S.
CORPORATE SOURCE: Department of Chemistry, North Carolina State University, Raleigh, NC, 27695-8204, USA

SOURCE: Journal of Organic Chemistry (**2002**), 67(11), 3811-3826
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

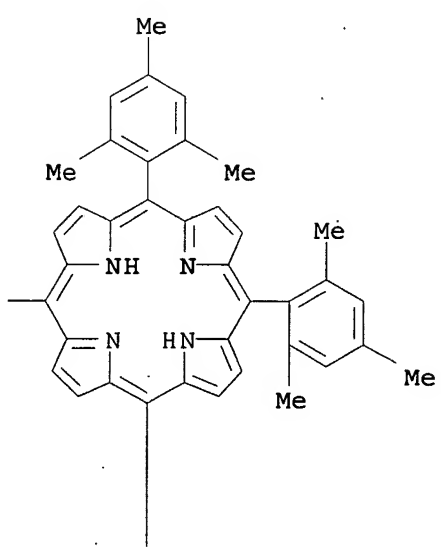
AB Mol. photonic wires, which absorb light and undergo excited-state energy transfer, are of interest as biomimetic models for photosynthetic light-harvesting systems and as **mol. devices** with potential applications in materials chemical The authors describe the stepwise synthesis of four mol. photonic wires. Each wire consists of an input unit, transmission element, and output unit. The input unit consists of a B-dipyrrin dye or a perylene-monoimide dye (linked either at the N-imide or the C9 position); the transmission element consists of one or three Zn porphyrins affording short or long wires, resp.; and the output unit consists of a free base (Fb) porphyrin. The components in the arrays are joined in a linear architecture via diarylethyne linkers (an ethynylphenyl linker is attached to the C9-linked perylene). The wires were examined by static absorption, static fluorescence, and time-resolved absorption spectroscopy. Each wire (with the exception of the C9-linked perylene wire) exhibits a visible absorption spectrum that is the sum of the spectra of the component parts, indicating the relatively weak electronic coupling between the components. Excitation of each wire at the wavelength where the input unit absorbs preferentially (typically 480-520 nm) results in emission almost exclusively from the Fb porphyrin. The static emission and time-resolved data indicate that the overall rate consts. and quantum efficiencies for end-to-end (i.e., input to output) energy transfer are as follows: perylene-(N-imide)-linked short wire, (33 ps)-1 and >99%; perylene-(C9)-linked short wire, (26 ps)-1 and >99%; B-dipyrrin-based long wire, (190 ps)-1 and 81%; perylene-(N-imide)-linked long wire, (175 ps)-1 and 86%. Collectively, the studies provide valuable insight into the singlet-singlet excited-state energy-transfer properties in weakly coupled mol. photonic wires.

CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related
Properties)
ST photonic wire excited state energy transfer porphyrin perylene
fluorescence; visible absorption porphyrin perylene photonic wire
IT Excited state
(singlet; synthesis and excited-state energy-transfer dynamics of
weakly coupled mol. photonic wires)
IT Energy transfer
Fluorescence
Photonics
UV and visible spectra
(synthesis and excited-state energy-transfer dynamics of weakly coupled
mol. photonic wires)
IT Optical absorption
(transient; synthesis and excited-state energy-transfer dynamics of
weakly coupled mol. photonic wires)
IT 150152-74-2 **160700-59-4** 165261-25-6 165550-61-8
180156-49-4 303089-28-3 303089-32-9 439798-40-0
RL: PRP (Properties)
(synthesis and excited-state energy-transfer dynamics of weakly coupled
mol. photonic wires)
IT **439798-32-0P 439798-33-1P** 439814-01-4P 439814-03-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and excited-state energy-transfer dynamics of weakly coupled
mol. photonic wires)
IT 160682-09-7 165261-51-8 180156-48-3 184154-12-9 439695-35-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and excited-state energy-transfer dynamics of weakly coupled
mol. photonic wires)
IT **439798-34-2P 439798-35-3P 439798-36-4P**
439798-37-5P 439798-38-6P 439798-39-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(synthesis and excited-state energy-transfer dynamics of weakly coupled
mol. photonic wires)
IT **160700-59-4**
RL: PRP (Properties)
(synthesis and excited-state energy-transfer dynamics of weakly coupled
mol. photonic wires)
RN 160700-59-4 HCAPLUS
CN Zinc, [10,15,20-tris(2,4,6-trimethylphenyl)-5-[4-[[4-[10,15,20-tris(2,4,6-
trimethylphenyl)-21H,23H-porphin-5-yl]phenyl]ethynyl]phenyl]-21H,23H-
porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-2)-
(9CI) (CA INDEX NAME)

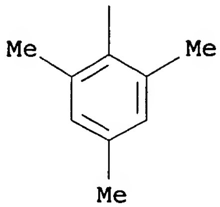
PAGE 1-A



PAGE 1-B



PAGE 2-B



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 23 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:90296 HCAPLUS
DOCUMENT NUMBER: 136:159162
TITLE: In situ regrowth and purification of crystalline thin films
INVENTOR(S): Liu, Chong-Yang; Bard, Allen J.
PATENT ASSIGNEE(S): Board of Regents, the University of Texas System, USA
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008500	A2	20020131	WO 2001-US22897	20010718 <--
WO 2002008500	A3	20020530		

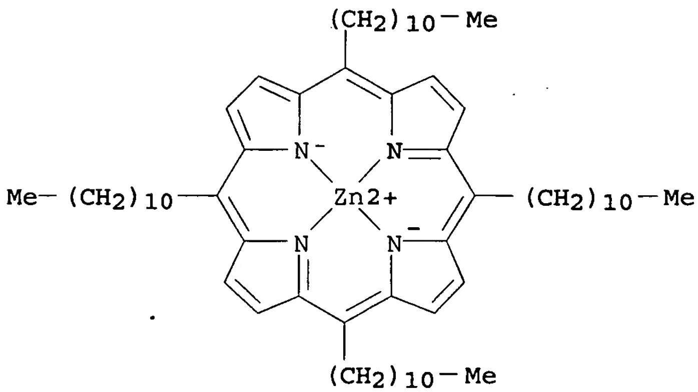
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2002033129	A1	20020321	US 2001-907546	20010716 <--
US 6840999	B2	20050111		

PRIORITY APPLN. INFO.: US 2000-220701P P 20000725 <--
US 2001-907546 A1 20010716 <--

AB Amorphous or polycryst. films were recrystd. into single-crystal thin films (of micrometer thickness) by a zone melting technique, in which an elec. heated wire generated a narrow heated or molten zone (0.5-2 mm wide) on the **substrate** sandwiched between 2 pieces of glass or In-Sn-oxide-coated glass. The **substrate** can be either an organic or inorg. compound When the molten zone was moved slowly (3-120 μm/min) across the layer form one end of the cell to the other, a single-crystal film was produced after a single pass. This technique allows for thin film purification and an improvement in electronic, optical, and optoelectronic properties of the thin film. After this treatment, the steady-state short-circuit photocurrent can be improved by several orders of magnitude.
IC ICM C30B013-00
CC 75-1 (Crystallography and Liquid Crystals)
Section cross-reference(s): **73**, 76
ST regrowth purifn cryst film zone melting

IT Photoelectric **devices**
(film; recrystn. by zone melting of amorphous or polycryst. films to enhance steady-state short-circuit photocurrent)
IT Vapor deposition process
(recrystn. by zone melting of amorphous or polycryst. films formed by)
IT Porphyrins
RL: PEP (Physical, engineering or chemical process); PUR (Purification or recovery); PYP (Physical process); TEM (Technical or engineered material use); PREP (Preparation); PROC (Process); USES (Uses)
(recrystn. by zone melting of amorphous or polycryst. films of)
IT Glass, uses
RL: **DEV (Device component use)**; USES (Uses)
(recrystn. of amorphous or polycryst. films by zone melting using sample holder including flat surfaces of glass coated with indium tin-oxide)
IT Zone crystallization
(recrystn.; in situ regrowth and purification of crystalline thin films by)
IT Coating process
(spin; recrystn. by zone melting of amorphous or polycryst. films formed by)
IT Evaporation
(thermal; recrystn. by zone melting of amorphous or polycryst. films formed by)
IT 7440-06-4, Platinum, uses 273921-59-8, Nichrome
RL: **DEV (Device component use)**; USES (Uses)
(in situ regrowth and purification of crystalline thin films by zone melting using heating source of wire of)
IT 17354-14-2P, 1,4-Bis(butylamino)-9,10-anthraquinone **61646-26-2P**
209909-33-1P
RL: PEP (Physical, engineering or chemical process); PUR (Purification or recovery); PYP (Physical process); TEM (Technical or engineered material use); **PREP (Preparation)**; PROC (Process); USES (Uses)
(recrystn. by zone melting of amorphous or polycryst. films of)
IT 50926-11-9, Indium tin-oxide
RL: **DEV (Device component use)**; USES (Uses)
(recrystn. of amorphous or polycryst. films by zone melting using sample holder including flat surfaces of glass coated with indium tin-oxide)
IT **61646-26-2P**
RL: PEP (Physical, engineering or chemical process); PUR (Purification or recovery); PYP (Physical process); TEM (Technical or engineered material use); **PREP (Preparation)**; PROC (Process); USES (Uses)
(recrystn. by zone melting of amorphous or polycryst. films of)
RN 61646-26-2 HCAPLUS
CN Zinc, [5,10,15,20-tetraundecyl-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



L47 ANSWER 24 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:891137 HCAPLUS
DOCUMENT NUMBER: 136:301602
TITLE: Synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs
AUTHOR(S): del Rosario Benites, Maria; Johnson, Thomas E.; Weghorn, Steven; Yu, Lianhe; Rao, Polisetti Dharma; Diers, James R.; Yang, Sung Ik; Kirmaier, Christine; Bocian, David F.; Holten, Dewey; Lindsey, Jonathan S.
CORPORATE SOURCE: Department of Chemistry, North Carolina State University, Raleigh, NC, 27695-8204, USA
SOURCE: Journal of Materials Chemistry (**2002**), 12(1), 65-80
CODEN: JMACEP; ISSN: 0959-9428
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A convergent synthesis employing porphyrin building blocks has afforded dendrimeric multiporphyrin arrays containing n Zn-porphyrins (n = 4, 8, or 20) and one free base- (Fb-) porphyrin joined via diarylethyne linkers. Size exclusion chromatog. was used extensively for purification The arrays have sufficient solubility in toluene or other solvents for routine handling. With increasing size, the intense near-UV Soret ($S0 \rightarrow S2$) absorption band broadens, splits, and red shifts due to inter-porphyrin exciton coupling. In contrast, the weaker visible bands ($S0 \rightarrow S1$) remain essentially unchanged in position or width in proceeding from the monomer all the way to the 21-mer; however, the mol. extinction coeffs. of the visible bands scale with the number of porphyrins. Similarly, the one-electron oxidation potentials of the porphyrins are virtually unchanged as the arrays get larger. These results are indicative of relatively weak (but significant) electronic coupling between ground states and between the photophys. relevant lowest-excited-singlet states of the diarylethyne-linked porphyrins; thus, the characteristic properties of the individual units are retained as the architectures increase in complexity. Efficient excited-singlet-state energy transfer occurs among the Zn-porphyrins and ultimately to the sole Fb-porphyrin in each of the arrays, with the overall arrival time of energy at the trapping site increasing modestly with the number of Zn-porphyrins = 1 (45 ps), 2 (90 ps), 8 (105 ps), and 20 (220 ps). The overall energy-transfer efficiencies are 98%, 96%, 96%, and 92% in the same series. The ground-state hole-storage properties of the 21-mer (Zn20Fb) were examined Bulk electrolysis indicates that 21 (or more)

electrons can be removed from this array (e.g., one hole resides on each porphyrin) to yield a stable "super-charged" π-cation radical. Taken together, these results indicate that the convergent building-block synthesis approach affords dendrimeric multiporphyrin arrays with favorable properties for light-harvesting and hole storage.

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 11, 76

ST dendrimeric multiporphyrin porphyrin light harvesting array synthesis hole storage; energy transfer dendrimeric multiporphyrin porphyrin light harvesting array

IT UV and visible spectra
(absorption; synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs)

IT Molecular structure-property relationship
(adsorption; synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs)

IT Singlet state
(singlet-singlet energy transfer; synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs)

IT Energy transfer
(singlet-singlet; synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs)

IT Chromatography
(size exclusion; synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs)

IT Electrochemistry
(spectroelectrochem.; synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs)

IT **Molecular** electronic **devices**
Photosynthesis, artificial
(synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs in relation to)

IT Optical absorption
(transient; synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs)

IT **183281-31-4P** 409060-71-5P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs)

IT 29162-74-1 150152-74-2 159152-18-8 160682-10-0 160682-16-6 184154-12-9
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs)

IT **247163-44-6P** **408504-85-8P** 409060-48-6P 409060-49-7P 409060-52-2P 409060-53-3P 409060-72-6P 409060-74-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs)

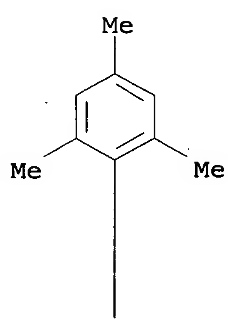
IT **183281-31-4P**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirs)

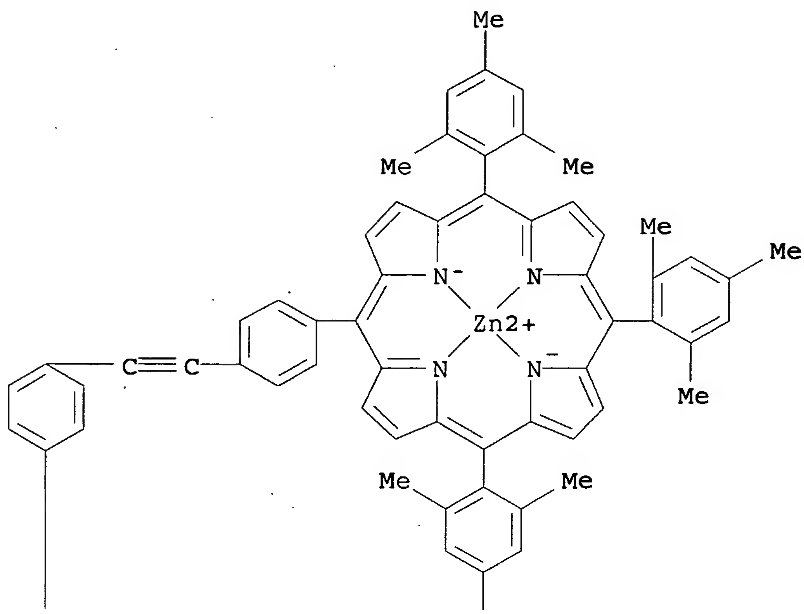
RN 183281-31-4 HCAPLUS

CN Zinc, [μ4-[5-(4-ethynyl-2,6-dimethylphenyl)-10,15,20-tris[4-[[4-[10,15,20-tris(2,4,6-trimethylphenyl)-21H,23H-porphin-5-yl-κN21,κN22,κN23,κN24]phenyl]ethynyl]phenyl]-21H,23H-porphinato(8-)-κN21,κN22,κN23,κN24]]tetra- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



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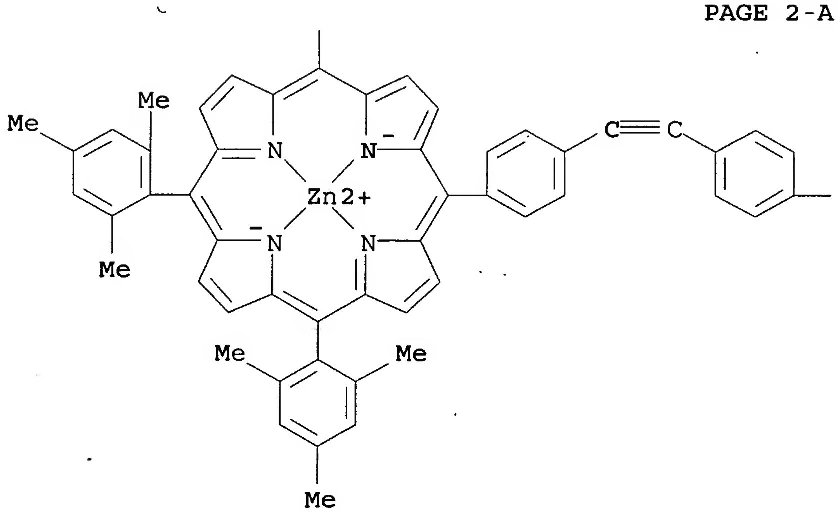

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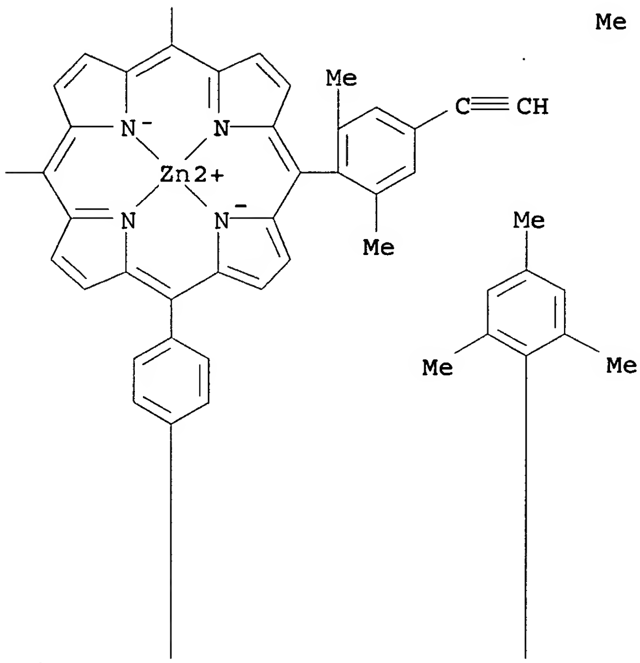

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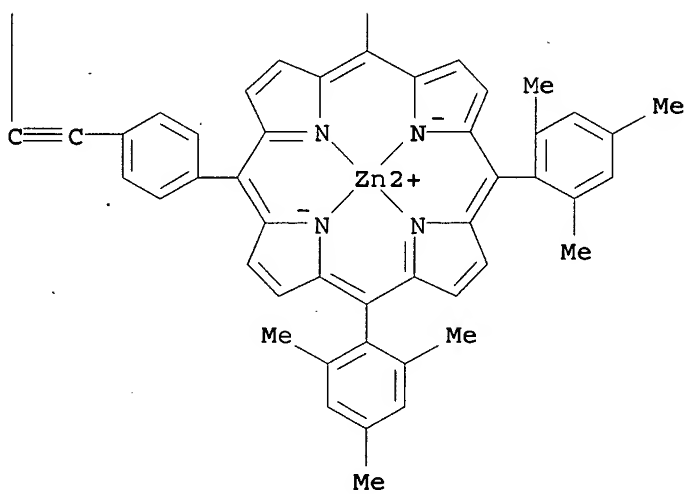


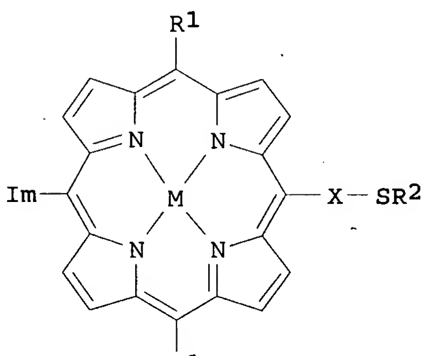
REFERENCE COUNT: 94 THERE ARE 94 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 25 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:681415 HCAPLUS
DOCUMENT NUMBER: 135:257635
TITLE: Mercapto-substituted **imidazolylporphyrin** -metal complex monomers, their **polymers**, and their preparation
INVENTOR(S): Kofuya, Yoshiaki; Ogawa, Kazuya

PATENT ASSIGNEE(S): Nara Advanced Science Technology Institute, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
JP 2001253883	A2	20010918	JP 2000-68766		20000313	<--
JP 3383839	B2	20030310				
US 2001027252	A1	20011004	US 2001-802923		20010312	<--
US 6602998	B2	20030805				
PRIORITY APPLN. INFO.:			JP 2000-68766	A	20000313	<--

OTHER SOURCE(S): MARPAT 135:257635
GI



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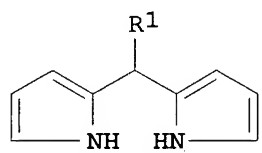

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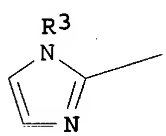
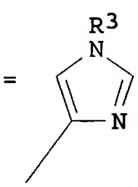
Q1 = 

Q2 = 

AB The monomers I [R1 = alkyl, aryl, alkyl(oxy)aryl; M = Zn, Ga, Ru, Fe, and/or Co; X = arylene- and/or alkylene-containing bivalent bridges; R2 = H, acetyl; Im = Q1, Q2 (R3 = H, alkyl)], dimers of I (II), **polymers** with 2 mercapto terminals (Markush given), and **polymers** with 1 mercapto and 1 quinonyl terminals (Markush given) are claimed. Also claimed are preparation process for I by (i) reaction of ImCHO, R2SXCHO, and III in the presence of TFA and (ii) insertion reaction of center metals in the resulted porphyrin derivs., where the whole process is carried out in the absence of coordinating solvents. The I are prepared by dissoln. of dimers II in coordinating solvents. The **polymers** with 2 mercapto terminals are prepared by dissoln. of II and poly(imidazolylporphyrin) (Markush given) in coordinating solvents followed by partial replacement of the solvents with noncoordinating solvents. The **polymers** with 1 mercapto and 1 quinonyl terminals

are prepared by mixing of one-mercapto-terminated poly(imidazolylporphyrin) (Markush given) with imidazolylporphyrin-quinonylporphyrin dimers (Markush given) in the presence of coordinating solvents. These **polymers** are useful for **mol.** wires, photoelec. **devices**, electron transfer media, and for artificial photosynthesis.

IC ICM C07D487-22
ICS C08G079-00; H01B001-12; H01L031-04

CC 35-8 (Chemistry of Synthetic High **Polymers**)
Section cross-reference(s): 26, 38

ST mercapto terminated **imidazolylporphyrin** zinc complex **polymer**; quinonyl mercapto terminated polyimidazolylporphyrin artificial photosynthesis; electron transport system polyimidazolylporphyrin zinc complex

IT **Polymers**, properties
RL: PRP (Properties)
(coordination; mercapto-substituted **imidazolylporphyrin**-metal complex derivs. for photoelec. devices and electron transport systems)

IT Chemical chains
Electron transport system, biological
Photoelectric devices
Photosynthesis, artificial
Solar cells
(mercapto-substituted imidazolylporphyrin-metal complex derivs. for photoelec. devices and electron transport systems)

IT Metalloporphyrins
RL: PNU (Preparation, unclassified); PRP (Properties); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(mercapto-substituted imidazolylporphyrin-metal complex derivs. for photoelec. devices and electron transport systems)

IT 67-56-1, Methanol, uses
RL: NUU (Other use, unclassified); USES (Uses)
(coordinating solvents; mercapto-substituted imidazolylporphyrin-metal complex derivs. for photoelec. devices and electron transport systems)

IT 361526-13-8P 361526-14-9P 361526-15-0P 361526-16-1P 361526-19-4P **361526-20-7P**
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(in preparation of imidazolylporphyrin-quinonylporphyrin dimer zinc complexes)

IT 50-00-0, Formaldehyde, reactions 84-58-2, Dichlorodicyanobenzoquinone 93-02-7, 2,5-Dimethoxybenzaldehyde **361526-18-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of imidazolylporphyrin-quinonylporphyrin dimer zinc complexes)

IT 76-05-1, Trifluoroacetic acid, uses
RL: CAT (Catalyst use); USES (Uses)
(in preparation of mercapto-terminated imidazolylporphyrin metal complex dimers)

IT 361526-12-7P
RL: PNU (Preparation, unclassified); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(in preparation of mercapto-terminated imidazolylporphyrin metal complex dimers)

IT 361526-11-6P
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(in preparation of mercapto-terminated imidazolylporphyrin metal complex dimers)

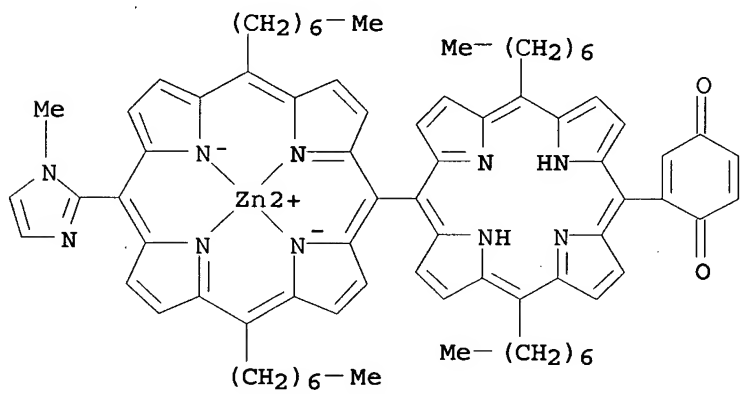
IT 557-34-6, Zinc acetate 13750-81-7 28130-89-4 352670-53-2
RL: RCT (Reactant); RACT (Reactant or reagent)

(in preparation of mercapto-terminated imidazolylporphyrin metal complex dimers)

IT 67-66-3, Chloroform, uses
RL: NUU (Other use, unclassified); USES (Uses)
(noncoordinating solvents; mercapto-substituted imidazolylporphyrin-metal complex derivs. for photoelec. devices and electron transport systems)

IT **361526-20-7P**
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(in preparation of imidazolylporphyrin-quinonylporphyrin dimer zinc complexes)

RN 361526-20-7 HCAPLUS
CN Zinc, [2-[10,10',20,20'-tetraheptyl-15'-(1-methyl-1H-imidazol-2-yl)[5,5'-bi-21H,23H-porphin]-15-yl-κN21',κN22',κN23',κN24']-2,5-cyclohexadiene-1,4-dionato(2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



L47 ANSWER 26 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:412540 HCAPLUS
DOCUMENT NUMBER: 135:152407
TITLE: Chiral Recognition by CD-Sensitive Dimeric Zinc Porphyrin Host. 1. Chiroptical Protocol for Absolute Configurational Assignments of Monoalcohols and Primary Monoamines
AUTHOR(S): Kurtan, Tibor; Nesnas, Nasri; Li, Yuan-Qiang; Huang, Xuefei; Nakanishi, Koji; Berova, Nina
CORPORATE SOURCE: Department of Chemistry, Columbia University, New York, NY, 10027, USA
SOURCE: Journal of the American Chemical Society (**2001**), 123(25), 5962-5973
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:152407

AB A general microscale protocol for the determination of absolute configurations of
primary amino groups or secondary hydroxyl groups linked to a single stereogenic center is described. The chiral **substrates** are linked to the achiral trifunctional bidentate carrier mol. (3-aminopropylamino)acetic acid (1, H2NCH2CH2CH2NHCH2COOH) and the resultant conjugates are then complexed with a dimeric Zn porphyrin host

tweezer complex 2 giving rise to 1:1 host/guest sandwiched complexes. These complexes exhibit exciton-coupled bisignate CD spectra due to stereodifferentiation leading to preferred porphyrin helicity. Since the chiral sense of twist between the two porphyrins in the complex is dictated by the stereogenic center of the **substrate**, the sign of the couplet dets. the absolute configuration at this center. The twist of the porphyrin tweezer in the complex can be predicted from the relative steric sizes of the groups flanking the stereogenic center, such that the bulkier group protrudes from the complex sandwich. In certain α-hydroxy esters and α-amino esters, electronic factors and H bonding govern the preferred conformation of the complex, and hence the CD spectra.

CC 22-3 (Physical Organic Chemistry)
Section cross-reference(s): **73**, 78

ST chiral recognition amine alc dimeric zinc porphyrin tweezer; CD dimeric zinc porphyrin tweezer chiral guest; reporter group CD dimeric zinc porphyrin tweezer; primary amine abs configuration zinc porphyrin tweezer deriv; secondary alc abs configuration zinc porphyrin tweezer deriv; abs configuration primary amine secondary alc

IT Absolute configuration
Chiral recognition
Circular dichroism
(absolute configuration of primary amine or secondary alc. determined from CD spectra of bidentate conjugate derivative with dimeric zinc porphyrin tweezer complex)

IT Exciton
(coupling; absolute configuration of primary amine or secondary alc. determined from CD spectra of bidentate conjugate derivative with dimeric zinc porphyrin tweezer complex)

IT Amines, reactions
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(primary, chiral; absolute configuration of primary amine or secondary alc. determined from CD spectra of bidentate conjugate derivative with dimeric zinc porphyrin tweezer complex)

IT Alcohols, reactions
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(secondary, chiral; absolute configuration of primary amine or secondary alc. determined from CD spectra of bidentate conjugate derivative with dimeric zinc porphyrin tweezer complex)

IT 109-76-2, 1,3-Diaminopropane
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-Boc protection of)

IT 53-41-8 464-45-9 521-18-6 599-04-2 697-64-3 1445-91-6
1517-66-4 2185-02-6 2216-51-5 2216-54-8 2627-86-3 4221-99-2
10065-72-2 10277-74-4 14898-79-4 14898-86-3 15914-84-8
17430-98-7 20698-91-3 23283-97-8 23357-52-0 24347-63-5
24915-95-5 27544-18-9 27871-49-4 34701-33-2 52019-78-0
52079-23-9 53732-47-1 60410-16-4 61866-20-4 94199-26-5
98919-68-7 99636-32-5 114446-55-8 249297-73-2 291523-12-1
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(absolute configuration determined from CD spectra of bidentate conjugate derivative with dimeric zinc porphyrin tweezer complex)

IT 80-97-7 516-95-0 15291-75-5 352284-60-7
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(absolute configuration of alc. center determined from CD spectra of bidentate

conjugate derivative with dimeric zinc porphyrin tweezer complex)
IT **352284-78-7P 352284-79-8P 352284-80-1P**
352284-81-2P 352284-82-3P 352284-83-4P
352284-90-3P 352284-91-4P 352284-92-5P
352284-93-6P 352284-94-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(absolute configuration of primary amine precursor determined from CD
spectra
of)
IT **352284-61-8P 352284-62-9P 352284-63-0P**
352284-64-1P 352284-65-2P 352284-66-3P
352284-67-4P 352284-68-5P 352284-69-6P
352284-70-9P 352284-71-0P 352284-72-1P
352284-73-2P 352284-74-3P 352284-75-4P
352284-76-5P 352284-77-6P 352284-84-5P
352284-85-6P 352284-86-7P 352284-87-8P
352284-88-9P 352284-89-0P 352284-95-8P
352284-96-9P 352284-97-0P 352284-98-1P
352285-68-8P 352285-69-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(absolute configuration of secondary alc. precursor determined from CD
spectra
of)
IT 79-08-3, Bromoacetic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(intermediate for determination of absolute configuration of primary amine
precursor)
IT 73391-93-2P 193967-71-4P 197566-55-5P 352285-15-5P 352285-33-7P
352285-34-8P 352285-35-9P 352285-36-0P 352285-37-1P 352285-39-3P
352285-40-6P 352285-41-7P 352285-42-8P 352285-55-3P 352285-56-4P
352285-57-5P 352285-58-6P 352285-59-7P 352285-60-0P 352285-61-1P
352285-62-2P 352285-63-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(intermediate for determination of absolute configuration of primary amine
precursor)
IT **210769-64-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(intermediate for determination of absolute configuration of secondary alc.
precursor)
IT 33038-81-2P 55284-67-8P 179927-97-0P 180061-59-0P 352285-00-8P
352285-01-9P 352285-02-0P 352285-03-1P 352285-04-2P 352285-05-3P
352285-06-4P 352285-07-5P 352285-08-6P 352285-09-7P 352285-10-0P
352285-11-1P 352285-12-2P 352285-13-3P 352285-14-4P 352285-16-6P
352285-17-7P 352285-19-9P 352285-23-5P 352285-24-6P 352285-25-7P
352285-26-8P 352285-27-9P 352285-28-0P 352285-29-1P 352285-30-4P
352285-31-5P 352285-32-6P 352285-43-9P 352285-44-0P 352285-45-1P
352285-46-2P 352285-47-3P 352285-48-4P 352285-49-5P 352285-50-8P
352285-51-9P 352285-52-0P 352285-53-1P 352285-54-2P 352285-64-4P
352285-65-5P 352285-66-6P 352285-67-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(intermediate for determination of absolute configuration of secondary alc.
precursor)
IT 258332-57-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and N-Boc protection of)
IT 352284-59-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and base hydrolysis of)
IT 352284-48-1P 352284-50-5P 352284-51-6P 352284-53-8P 352284-55-0P 352284-58-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with dimeric zinc porphyrin tweezer complex for determination of absolute configuration of alc. precursor)
IT 75178-96-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling with Et bromoacetate)
IT 352284-52-7P 352284-54-9P 352284-57-2P 352284-99-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection for determination of absolute configuration of alc.
precursor)
IT 352284-56-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with chiral primary amine or secondary alc. for attempted determination of absolute configuration)
IT 192124-66-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with chiral primary amine or secondary alc. for determination of absolute configuration)
IT 105-36-2, Ethyl bromoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of)
IT 56602-33-6
RL: RGT (Reagent); RACT (Reactant or reagent)
(preparation of)
IT 616-79-5P, 5-Nitroanthranilic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction with chiral primary amine or secondary alc. for attempted determination of absolute configuration)
IT 260970-57-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with chiral primary amine or secondary alc. for determination of absolute
configuration)
IT **352284-78-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(absolute configuration of primary amine precursor determined from CD spectra
of)
RN 352284-78-7 HCAPLUS
CN Zinc, [μ-[2-[[3-(amino-κN)propyl]amino-κN]-N-[(1R)-1,2-dimethylpropyl]acetamide]][μ-[[1,5-pentanediyl bis[4-(10,15,20-triphenyl-21H,23H-porphin-5-yl-κN21,κN22,κN23,κN24)benzoato]](4-)]]di- (9CI) (CA INDEX NAME)

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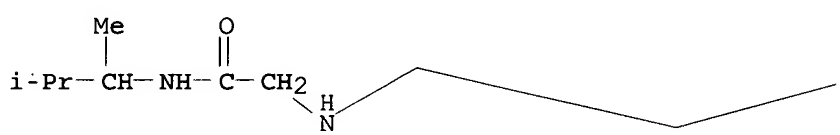

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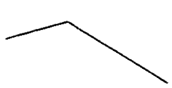

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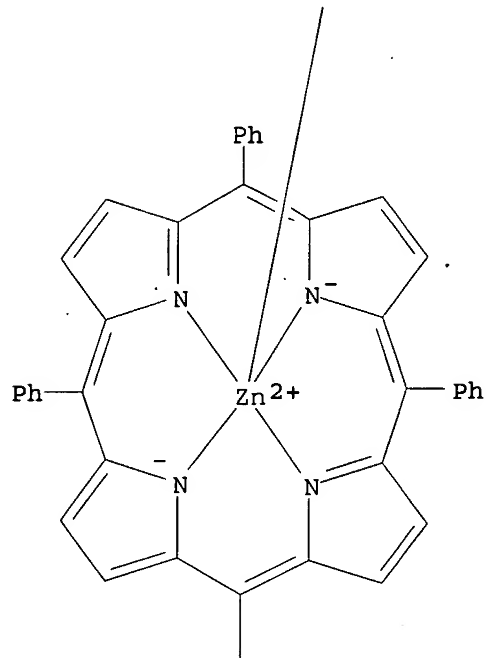

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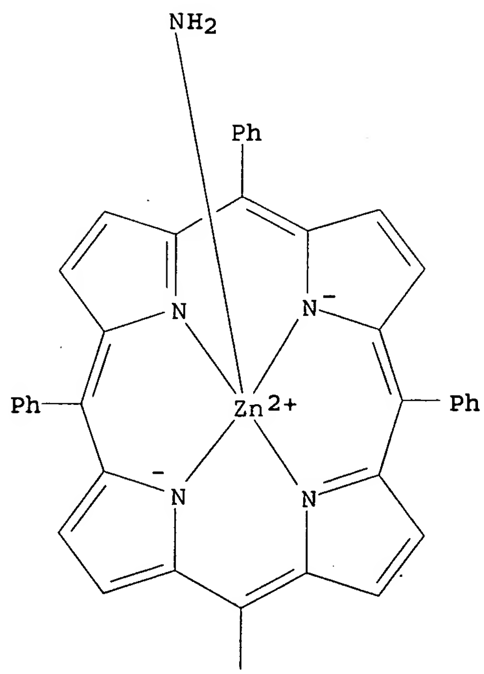
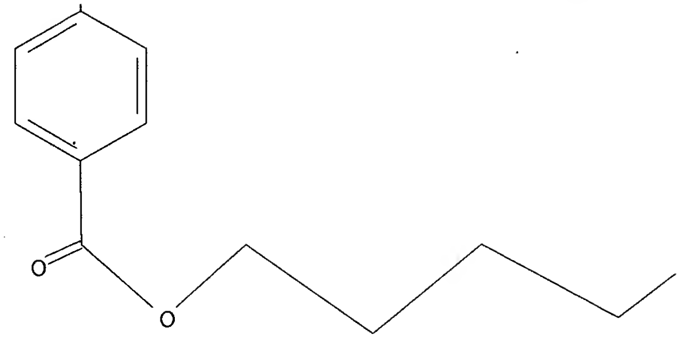


PAGE 3-A



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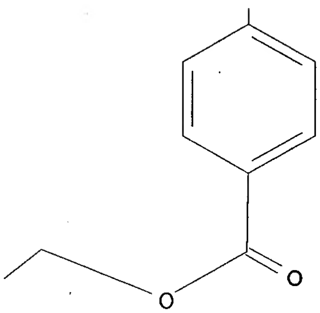


REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 27 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:293901 HCAPLUS
DOCUMENT NUMBER: 135:52986
TITLE: Excited-State Energy Transfer Processes in Phenylene- and Biphenylene-Linked and Directly-Linked Zinc(II) and Free-Base Hybrid Diporphyrins
AUTHOR(S): Cho, Hyun Sun; Jeong, Dae Hong; Yoon, Min-Chul; Kim, Yong Hee; Kim, Yong Rok; Kim, Dongho; Jeoung, Sae Chae; Kim, Seong Keun; Aratani, Naoki; Shinmori, Hideyuki; Osuka, Atsuhiro
CORPORATE SOURCE: Center for Ultrafast Optical Characteristics Control and Department of Chemistry, Yonsei University, Seoul, 120-749, S. Korea
SOURCE: Journal of Physical Chemistry A (**2001**), 105(17), 4200-4210
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The photoinduced energy transfer processes in 1,4-phenylene-, 1,3-phenylene, 1,2-phenylene, and 4,4'-biphenylene-linked and directly-linked Zn(II)-free base porphyrin heterodimers in THF were studied by femtosecond transient absorption spectroscopy. The energy transfer rates were compared between TPP-type and OEP-type heterodimers resp. as A2u-HOMO and A1u-HOMO subunits, for evaluating the relative

contribution of the through-bond and through-space interactions. The rate difference becomes smaller with a decrease of spacer, >10 for 1,4-bis(phenylethynyl)phenylene and 1,4-diphenylethynylene, 4 for 4,4'-biphenylene-linked heterodimer, and 3 for 1,3- and 1,4-phenylene-linked spacers. In the meso-meso directly-linked case, the energy transfer rates are the same ((0.55 ps)-1) for 5,5,15,15-tetrakis(3,5-bis(octyloxy)phenyl)-substituted and 5,5,15,15-tetrakis(pentafluorophenyl)-substituted heterodimers, featuring only a minor influence of the frontier orbital characteristics on the energy transfer rate. The energy transfer rates are identical (0.55 ps)-1 for the directly-linked meso-meso heterodimers substituted with 3,5-bis(octyloxy)phenyl and pentafluorophenyl groups regardless of the difference in the HOMO orbital symmetry characteristics, suggesting the predominant Coulombic interaction for the energy transfer in these close proximity porphyrin dimers. In the case of 1,2-phenylene-linked heterodimers, the choice of the peripheral substituents can lead to a state-to-state rapid energy transfer with a rate of (0.55 ps-1) for the TPP-type model or a delocalized excimer-like diporphyrin excited state for the OEP-type model. Collectively, these results indicate that even for the covalently-linked models the relative contribution of the through-space Coulombic interaction becomes increasingly important upon the decrease of the center-to-center separation Especially, the fast and efficient energy transfer occurring in the directly-linked heterodimer illustrates that this porphyrin unit can be used as a good candidate for energy transfer functional arrays in **mol.** photonic **devices.**

CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 26

ST excited state energy transfer phenylene biphenylene linked zinc diporphyrin

IT Intramolecular energy transfer
Photoinduced energy transfer
(excited-state energy transfer processes in phenylene- and biphenylene-linked and directly-linked zinc(II) and free-base hybrid diporphyrins)

IT Fluorescence
UV and visible spectra
(of phenylene- and biphenylene-linked and directly-linked zinc(II) and free-base hybrid diporphyrins)

IT Optical absorption
(transient; of phenylene- and biphenylene-linked and directly-linked zinc(II) and free-base hybrid diporphyrins)

IT 222620-15-7 344612-39-1
RL: PRP (Properties)
(emission spectra of zinc(II) and free-base porphyrins)

IT 205177-67-9 220355-87-3
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(emission spectra of zinc(II)-base porphyrins and synthesis of directly-linked zinc(II) and free-base hybrid diporphyrin using)

IT **128643-00-5 128667-08-3 128667-09-4**
160700-59-4 170707-84-3 199394-12-2
218155-84-1 237396-79-1 344738-39-2
344738-42-7
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(excited-state energy transfer processes in phenylene- and biphenylene-linked and directly-linked zinc(II) and free-base hybrid diporphyrins)

IT **96481-87-7P 344738-37-0P 344738-38-1P**

344738-40-5P 344738-41-6P 344738-43-8P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(synthesis and excited-state energy transfer processes in phenylene- and biphenylene-linked and directly-linked zinc(II) and free-base hybrid diporphyrins)

IT 66-98-8, [1,1'-Biphenyl]-4,4'-dicarboxaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis intermediate of biphenylene-linked zinc(II) and free-base hybrid diporphyrin prepared using)

IT 132911-80-9P **205177-68-0P 276867-69-7P** 344612-41-5P 344612-44-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis intermediate of biphenylene-linked zinc(II) and free-base hybrid diporphyrins)

IT 125187-60-2P 216306-28-4P 344612-42-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis intermediate of phenylene-linked zinc(II) and free-base hybrid diporphyrin)

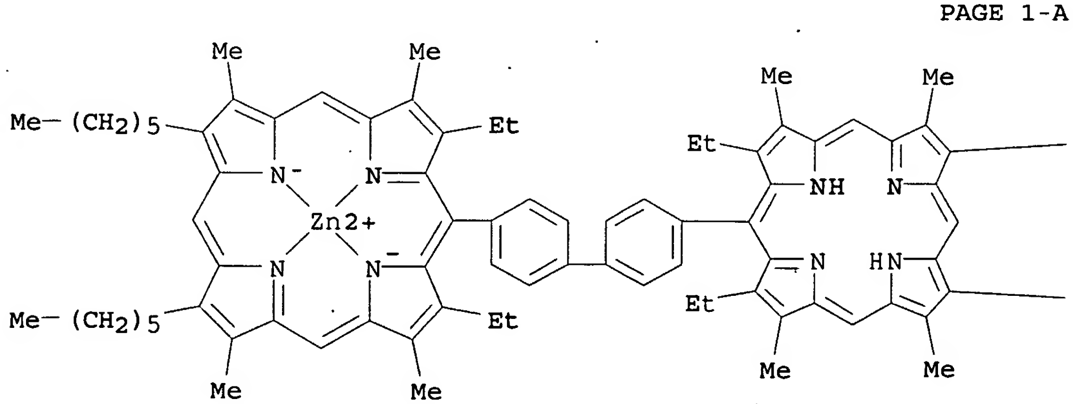
IT 100-52-7, Benzaldehyde, reactions 623-27-8, Terephthalaldehyde 626-19-7, 1,3-Benzenedicarboxaldehyde 17610-00-3 34046-43-0 107798-98-1 181762-72-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis intermediate of phenylene-linked zinc(II) and free-base hybrid diporphyrin prepared using)

IT 82873-90-3P 129496-68-0P 344612-40-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis intermediate of phenylene-linked zinc(II) and free-base hybrid diporphyrins)

IT **128643-00-5**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(excited-state energy transfer processes in phenylene- and biphenylene-linked and directly-linked zinc(II) and free-base hybrid diporphyrins)

RN 128643-00-5 HCAPLUS
CN Zinc, [5-[4'-(3,7-diethyl-13,17-dihexyl-2,8,12,18-tetramethyl-21H,23H-porphin-5-yl)[1,1'-biphenyl]-4-yl]-3,7-diethyl-13,17-dihexyl-2,8,12,18-tetramethyl-21H,23H-porphinato(2-)-κN21,κN22,κN23,.kappa .N24]-, (SP-4-2)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— $(CH_2)_5$ — Me

— $(CH_2)_5$ — Me

REFERENCE COUNT: 82 THERE ARE 82 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 28 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:667679 HCAPLUS
DOCUMENT NUMBER: 133:357171
TITLE: Investigation of Tightly Coupled Porphyrin Arrays Comprised of Identical Monomers for Multibit Information Storage
AUTHOR(S): Clausen, Christian; Gryko, Daniel T.; Yasseri, Amir A.; Diers, James R.; Bocian, David F.; Kuhr, Werner G.; Lindsey, Jonathan S.
CORPORATE SOURCE: Department of Chemistry, North Carolina State University, Raleigh, NC, 27695-8204, USA
SOURCE: Journal of Organic Chemistry (**2000**), 65(22), 7371-7378
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors prior designs for **mol.**-based information storage **devices** have employed multiple redox-active units organized in weakly coupled, covalently linked arrays. To explore a simpler design, the authors report the synthesis of porphyrin arrays where porphyrins with identical oxidation potentials are directly linked to one another instead of joined via a mol. linker. Oxidative coupling with AgPF6 of zinc(II)-5,15-bis(4-tert-butylphenyl)-10-phenylporphyrin, obtained by a rational synthesis, afforded the expected dimer joined by a meso-meso linkage and an unexpected trimer joined by meso-meso linkages. For attachment to an electroactive surface the authors synthesized a meso-linked porphyrin dimer with a thiol-linker in one of the meso positions. The S-acetyl protecting group was used to avoid handling free thiol groups. Coupling of zinc(II)-5,10,15-tris(3,5-di-tert-butylphenyl)porphyrin ("upper half") and zinc(II)-5-[4-(S-acetylthio)phenyl]-10,20-bis(3,5-di-tert-butylphenyl)porphyrin ("lower half") afforded three different meso-linked dimers with the desired dimer as the main product. Electrochem. examination of the meso-linked dimer in solution shows that the first two oxidation potentials of the array differ by .apprx.0.15 V and straddle the value exhibited by the monomeric constituents. The third and fourth oxidation potentials of the array are also split although to a lesser extent (.apprx.0.08 V) than the first and second. For the meso-linked trimer, the first three oxidation waves are also split; however, these waves are severely overlapped. The electrochem. behavior of the dimers and trimer is indicative of strong electronic interactions among the porphyrins. The thiol-derivatized meso-linked

dimers form self-assembled monolayers (SAMs) on gold via in situ cleavage of the S-acetylthio protecting group. The porphyrin SAM exhibits four well-resolved oxidation waves. Regardless, the meso-meso linkage is relatively unstable upon formation of the π-cation radical(s). This characteristic indicates that the structural motif is of limited utility for mol. information storage elements.

CC 74-12 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 26, 72, 78

ST synthesis electrochem property porphyrin array multibit information storage

IT Self-assembly
(electrochem. of tightly-coupled porphyrin arrays in solution and in self-assembled monolayer for multibit information storage)

IT Memory devices
(electrochem. of tightly-coupled porphyrin arrays in solution and in self-assembled monolayer for multibit information storage in relation to)

IT Redox reaction
(electrochem.; electrochem. of tightly-coupled porphyrin arrays in solution and in self-assembled monolayer for multibit information storage)

IT Oxidation potential
Oxidation potential
(half-wave; electrochem. of tightly-coupled porphyrin arrays in solution and in self-assembled monolayer for multibit information storage)

IT Half wave potential
Half wave potential
(oxidation; electrochem. of tightly-coupled porphyrin arrays in solution and in self-assembled monolayer for multibit information storage)

IT Information systems
(storage; electrochem. of tightly-coupled porphyrin arrays in solution and in self-assembled monolayer for multibit information storage in relation to)

IT Metalloporphyrins
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(zinc complexes; of porphyrin arrays where porphyrins with identical oxidation potentials are directly linked to one another and their building blocks)

IT 7440-57-5, Gold, uses
RL: NUU (Other use, unclassified); USES (Uses)
(electrochem. of tightly-coupled porphyrin arrays in self-assembled monolayers attached to gold surface for multibit information storage)

IT **201593-21-7P 305830-94-8P 305830-95-9P**
305831-02-1P 305831-03-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(electrochem. properties and synthesis of porphyrin arrays where porphyrins with identical oxidation potentials are directly linked to one another for multibit information storage)

IT 3109-63-5, Tetrabutylammonium hexafluorophosphate
RL: NUU (Other use, unclassified); USES (Uses)
(electrolyte; electrochem. of tightly-coupled porphyrin arrays in solution and in self-assembled monolayer for multibit information storage)

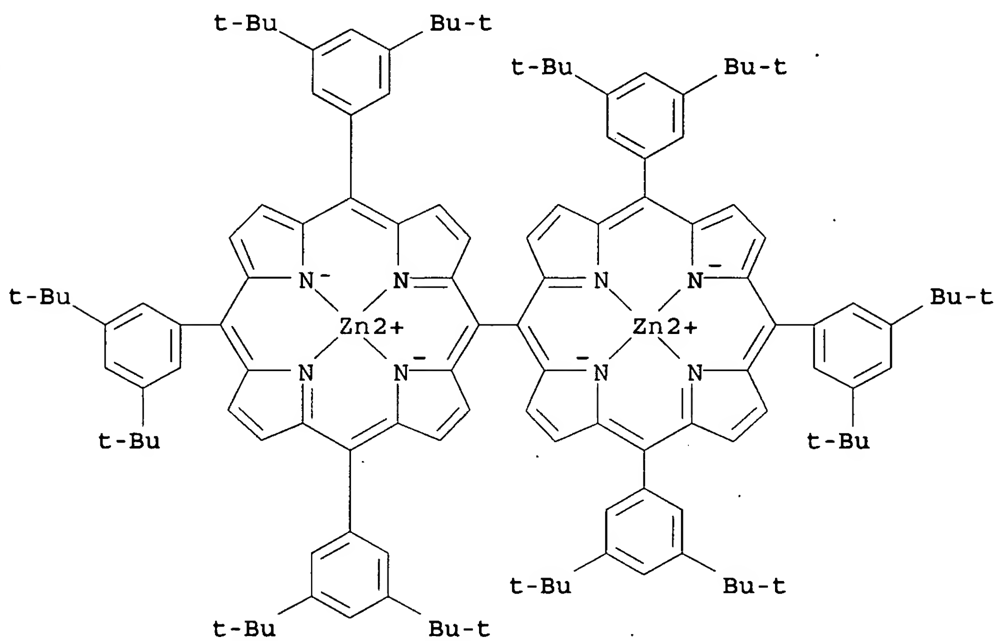
IT 201593-15-9P 259194-41-7P 305830-91-5P 305830-92-6P 305830-93-7P
305830-96-0P 305830-97-1P 305830-98-2P 305830-99-3P 305831-00-9P
305831-01-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of porphyrin arrays where porphyrins with identical oxidation potentials are directly linked to one another)

IT **201593-21-7P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(electrochem. properties and synthesis of porphyrin arrays where porphyrins with identical oxidation potentials are directly linked to one another for multibit information storage)

RN   201593-21-7   HCAPLUS

CN   Zinc, [μ-[10,10',15,15',20,20'-hexakis[3,5-bis(1,1-dimethylethyl)phenyl]-5,5'-bi-21H,23H-porphinato(4-)-κN21,κN22,κN23,κN24:κN21',κN22',.kappa.N23',κN24']]di- (9CI)   (CA INDEX NAME)



REFERENCE COUNT: 23   THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 29 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:664047 HCAPLUS
DOCUMENT NUMBER: 133:368750
TITLE: Three-dimensionally arranged windmill and grid porphyrin arrays by AgI-promoted meso-meso block oligomerization
AUTHOR(S):   Nakano, Aiko; Yamazaki, Tomoko; Nishimura, Yoshinobu; Yamazaki, Iwao; Osuka, Atsuhiro
CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, Kyoto University, Kyoto, 606-8502, Japan
SOURCE: Chemistry--A European Journal (2000), 6(17), 3254-3271
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S):   CASREACT 133:368750

AB   The syntheses of soluble windmill and grid porphyrin arrays through the AgI-promoted coupling reaction of 1,4-phenylene-bridged linear porphyrin arrays, which are comprised of a central ZnII β-free porphyrin and flanking peripheral NiII β-octaalkylporphyrins, are described. The

coupling reaction is advantageous in light of its high regioselectivity occurring only at the meso-position of the ZnII β-free porphyrin as well as its easy extension to large porphyrin arrays. The windmill porphyrin arrays in turn serve as an effective **substrate** for further coupling reactions, to give three-dimensionally arranged grid porphyrin arrays. Further the grid porphyrin 12-mer (a tetramer of the linear porphyrin trimer) was also coupled to afford grid porphyrins (24-mer, 36-mer, and 48-mer). These porphyrin arrays were isolated in a discrete form by repetitive GPC/HPLC (GPC = gel-permeation chromatog.). Competitive expts. with three linear porphyrin trimers bearing different peripheral metalloporphyrins (ZnII, NiII, and CuII), and the trapping experiment of the radical cation at the peripheral porphyrin with AgNO2, suggested that an initial 1-electron oxidation of the easily oxidizable peripheral ZnII β-octaalkylporphyrin with an AgI ion and a subsequent endothermic hole transfer assist the generation of the radical cation at the central ZnII β-free porphyrin. In all ZnII-metalated windmill porphyrin arrays, the energy level of the S1 state of the meso - meso-linked diporphyrin core is lower than that of the peripheral porphyrins, thereby allowing an energy flow from the peripheral porphyrins to the central diporphyrin core; this was confirmed by measurements of fluorescence lifetimes and picosecond time-resolved fluorescence spectra. The excitation energy transfer in the arrays encourages their potential use as an light-harvesting antenna.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 72, **73**, 74

ST porphyrin transition metal extended array complex prepn; oxidn potential transition metal porphyrin complex

IT Coupling reaction
(in preparation of transition metal porphyrin extended array complexes)

IT Rotational barrier
(of transition metal porphyrin extended array complexes)

IT Energy transfer
Fluorescence
Physical process kinetics
(of zinc porphyrin extended array complexes)

IT Transition metal complexes
Transition metal complexes
RL: SPN (Synthetic preparation); PREP (Preparation)
(porphyrin; preparation of transition metal porphyrin extended array complexes)

IT Metalloporphyrins
Metalloporphyrins
RL: SPN (Synthetic preparation); PREP (Preparation)
(transition metal; preparation of transition metal porphyrin extended array complexes)

IT 219638-63-8P 219638-84-3P **307313-29-7P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and fluorescence)

IT **307313-34-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and nitration)

IT **219589-09-0P** **219589-14-7P** 219638-58-1P 219638-60-5P
219638-81-0P 219638-87-6P 307312-74-9P 307312-77-2P 307312-78-3P
307313-28-6P **307313-30-0P** **307313-31-1P**
307313-32-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactant for preparation of transition metal porphyrin extended

array complexes)

IT **219589-10-3P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactant for preparation of transition metal porphyrin extended array complexes and oxidation potentials)

IT **219589-15-8P** 219638-59-2P 219638-82-1P 219638-92-3P 307312-63-6P 307312-64-7P 307312-65-8P 307312-66-9P 307312-67-0P 307312-68-1P 307312-69-2P 307312-71-6P 307312-72-7P 307312-73-8P 307312-75-0P 307312-76-1P 307312-79-4P **307313-33-3P** **307313-35-5P** **307313-36-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

IT 26042-63-7, Silver hexafluorophosphate

RL: CAT (Catalyst use); USES (Uses)

(preparation of three-dimensionally arranged windmill and grid transition metal porphyrin arrays by AgI-promoted meso-meso block oligomerization)

IT 17610-00-3, 3,5-Di-tert-butylbenzaldehyde 21211-65-4, 2,2'-Dipyrrylmethane 219554-60-6 **307313-38-8** **307313-39-9**

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for preparation of transition metal porphyrin extended array complexes)

IT 219589-07-8 219589-08-9 307313-37-7

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)

(reactant for preparation of transition metal porphyrin extended array complexes and oxidation potential)

IT **307313-29-7P**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(preparation and fluorescence)

RN 307313-29-7 HCAPLUS

CN Zinc, [μ4-[10,10'-bis[3,5-bis(1,1-dimethylethyl)-20,20'-bis[4-[15-[4-[(2,5-dimethoxyphenyl)methyl]phenyl]-2,8,12,18-tetrahexyl-3,7,13,17-tetramethyl-21H,23H-porphin-5-yl-κN21,κN22,κN23,κN24]phenyl]-5,5'-bi-21H,23H-porphinato(8-)-κN21,κN22,κN23,κN24:κN21',κN22',κN23',κN24']]]tetra- (9CI) (CA INDEX NAME)

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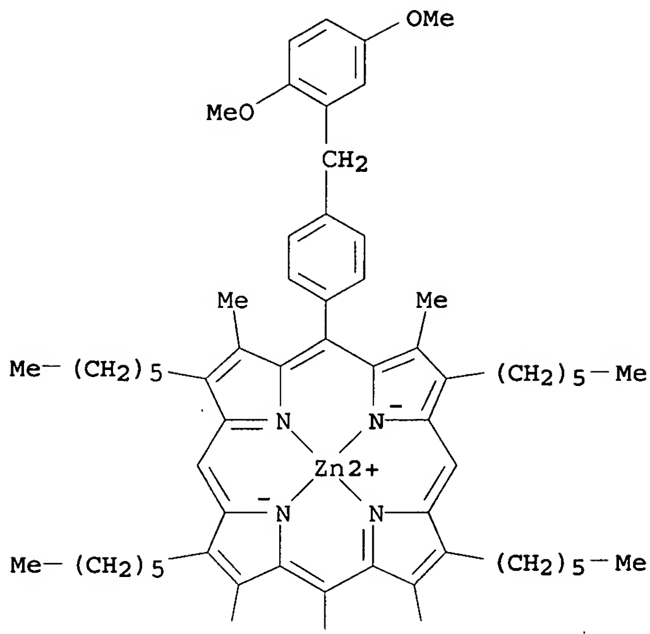

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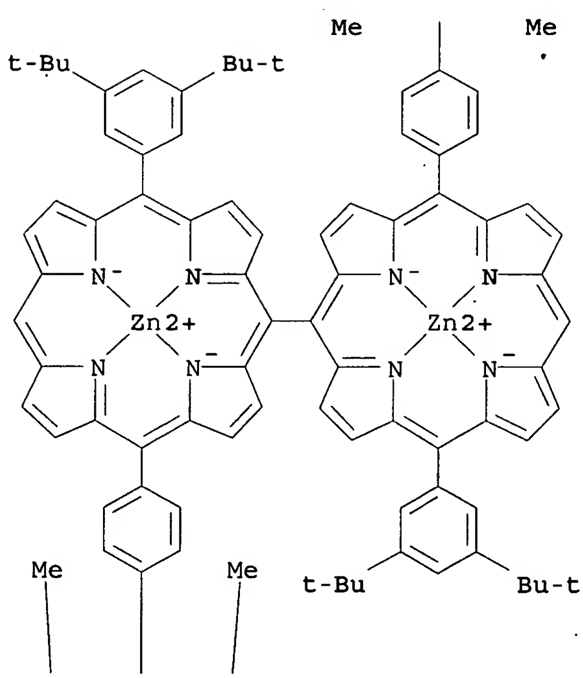

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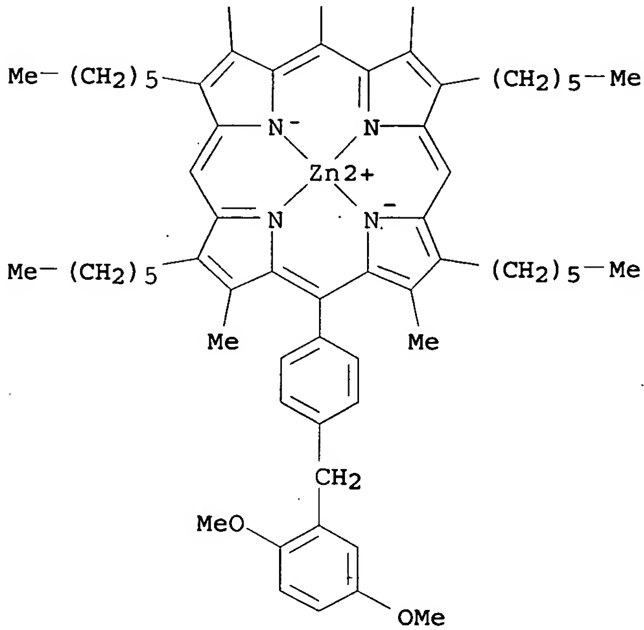


REFERENCE COUNT: 98 THERE ARE 98 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

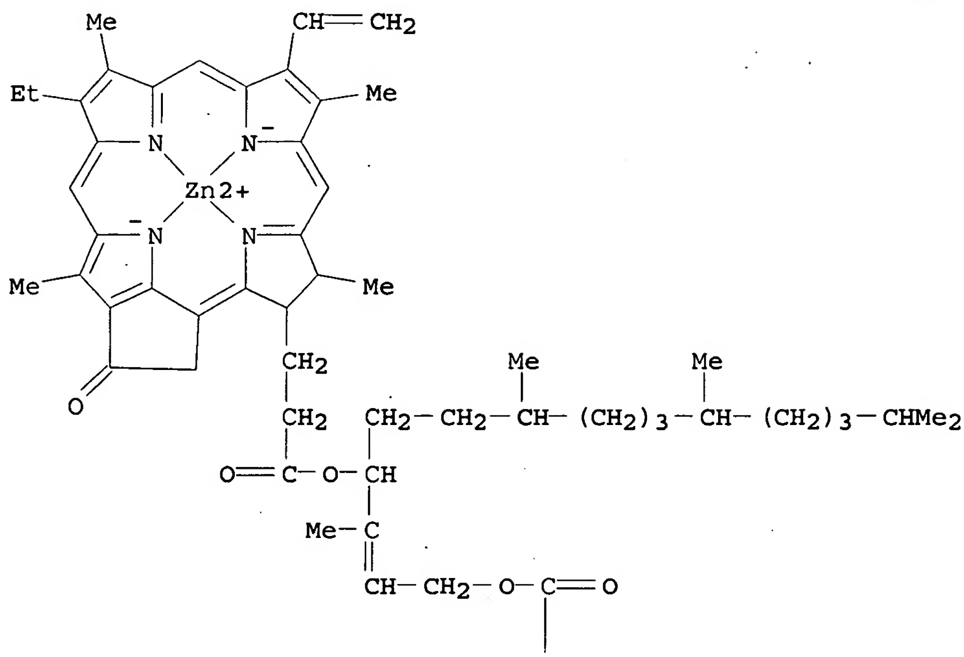
L47 ANSWER 30 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:656868 HCAPLUS
DOCUMENT NUMBER: 134:63367
TITLE: Photophysical studies of 1,4-diazabicyclo(2,2,2)octane as a bifunctional ligand to fix the conformation of a flexibly-linked phorbinato-zinc dimer
AUTHOR(S): Puranen, E.-L.; Stapelbroek-Mollmann, M. E.; Vuorimaa, E.; Tkachenko, N.; Tauber, A. Y.; Hynninen, P. H.; Lemmetyinen, H.
CORPORATE SOURCE: Institute of Materials Chemistry, Tampere University of Technology, Tampere, FIN-33101, Finland
SOURCE: Journal of Photochemistry and Photobiology, A: Chemistry (**2000**), 136(3), 179-184
CODEN: JPPCEJ; ISSN: 1010-6030
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The binding of a bifunctional ligand 1,4-diazabicyclo(2,2,2)octane (DABCO) to a phorbin-dimer (PP) in which a phytochlorin is covalently linked with a flexible spacer to a modified phytyl residue of pyropheophytin was studied in order to establish a rigid face-to-face intramol. dimer. Steady-state and time-resolved fluorescence and absorption spectroscopies were employed to characterize the binding equilibrium in CH2Cl2 and to verify the formation of a 1:1 complex where DABCO is bound between the Zn-phorbin rings of the dimer. The proportion of this complex is highest, about 88%, at the molar ratio of ligand:**substrate** = 1.5:1 while at higher molar ratios, a second DABCO mol. binds to the dimer breaking down the fixed complex.

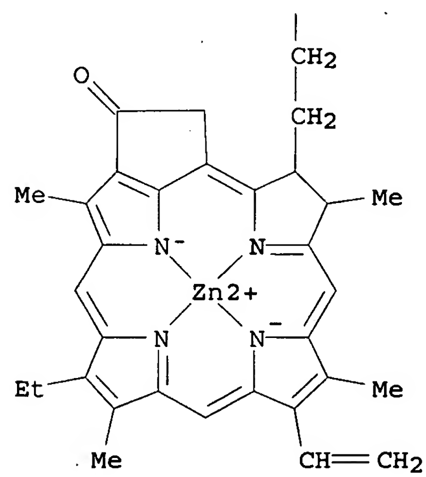
CC 73-5 (**Optical**, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 74, 78

ST photophysics DABCO zinc phorbin dimer; complexation DABCO zinc pyropheophytin dimer fluorescence
IT UV and visible spectra
(absorption; photophys. study of binding of bifunctional ligand DABCO to phorbin-dimer in which phytochlorin is covalently linked with flexible spacer to modified phytyl residue of pyropheophytin)
IT Absorption spectra
Complexation
Fluorescence
Formation constant
(photophys. study of binding of bifunctional ligand DABCO to phorbin-dimer in which phytochlorin is covalently linked with flexible spacer to modified phytyl residue of pyropheophytin)
IT Photoinduced electron transfer
(photophys. study of binding of bifunctional ligand DABCO to phorbin-dimer in which phytochlorin is covalently linked with flexible spacer to modified phytyl residue of pyropheophytin in relation to)
IT 110-86-1, Pyridine, properties
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(complexation of zinc phorbin-dimers with pyridine)
IT 280-57-9, DABCO
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(photophys. study of binding of bifunctional ligand DABCO to phorbin-dimer in which phytochlorin is covalently linked with flexible spacer to modified phytyl residue of pyropheophytin)
IT 15333-64-9 **313945-34-5** 313945-35-6 **313945-36-7**
313945-37-8
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(photophys. study of binding of bifunctional ligand DABCO to phorbin-dimer in which phytochlorin is covalently linked with flexible spacer to modified phytyl residue of pyropheophytin)
IT **313945-34-5**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(photophys. study of binding of bifunctional ligand DABCO to phorbin-dimer in which phytochlorin is covalently linked with flexible spacer to modified phytyl residue of pyropheophytin)
RN 313945-34-5 HCAPLUS
CN Zinc, [μ-[[(2E)-2-methyl-1-[(3R,7R)-3,7,11-trimethyldodecyl]-2-butene-1,4-diyl bis[(3S,4S)-9-ethenyl-14-ethyl-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato-κN23,κN24,κN25,κN26]](4-)]]di-
(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 31 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:496824 HCAPLUS
DOCUMENT NUMBER: 133:259179
TITLE: Structural Control of Photoinduced Energy Transfer between Adjacent and Distant Sites in Multiporphyrin Arrays

AUTHOR(S): Lammi, Robin K.; Ambroise, Arounaguiry; Balasubramanian, Thiagarajan; Wagner, Richard W.; Bocian, David F.; Holten, Dewey; Lindsey, Jonathan S.
CORPORATE SOURCE: Departments of Chemistry, Washington University, St. Louis, MO, 63130-4889, USA
SOURCE: Journal of the American Chemical Society (**2000**), 122(31), 7579-7591
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A family of diphenylethyne-linked porphyrin dimers and trimers has been prepared via a building block approach for studies of energy-transfer processes. The dimers contain Mg and Zn porphyrins (MgZnU); the trimers contain an addnl. free base porphyrin (MgZnFbU). In both the dimers and trimers, sites of attachment to the Mg porphyrin (at the meso- or β-position) and diphenylethyne linker (at the para- or meta-positions) were varied, producing four Mg porphyrin-Zn porphyrin arrangements with the following linker configurations: meso-p/p-meso, meso-m/p-meso, β-p/p-meso, and β-m/p-meso. All four trimers employ a meso-p/p-meso Zn porphyrin-Fb porphyrin connection. The ground- and excited-state properties of the porphyrin dimers and trimers have been examined using static and time-resolved optical techniques. The rate of energy transfer from the photoexcited Zn porphyrin to the Mg porphyrin decreases according to the following trend: meso-p/p-meso (9 ps)-1 > β-p/p-meso (14 ps)-1 > meso-m/p-meso (19 ps)-1 > β-m/p-meso (27 ps)-1. In each compound, energy transfer between adjacent porphyrins occurs through a linker-mediated through-bond process. The rate of energy transfer between Zn and Fb porphyrins is constant in each trimer ((24 ps)-1). Energy transfer from the photoexcited Zn porphyrin branches to the adjacent Fb and Mg porphyrins, with nearly one-half to three-fourths proceeding to the Mg porphyrin (depending on the linker). Energy transfer from the excited Mg porphyrin to the nonadjacent Fb porphyrin occurs more slowly, with a rate that follows the same trend in linker architecture and porphyrin connection site: meso-p/p-meso (173 ps)-1 > β-p/p-meso (225 ps)-1 > meso-m/p-meso (320 ps)-1 > β-m/p-meso (385 ps)-1. The rate of transfer between nonadjacent Mg and Fb porphyrins does not change significantly with temperature, indicating a superexchange mechanism utilizing orbitals/states on the intervening Zn porphyrin. Energy transfer between nonadjacent sites may prove useful in directing energy flow in multiporphyrin arrays and related **mol.** photonic **devices**

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 76
ST photoinduced energy transfer mechanism zinc magnesium porphyrin array; multiporphyrin zinc magnesium array photoinduced energy transfer kinetics
IT UV and visible spectra
(absorption; photoinduced energy transfer in diphenylethyne-linked dimers containing Mg- and Zn porphyrin units and trimers containing addnl. free-base unit)
IT Photoinduced energy transfer
(kinetics; photoinduced energy transfer in diphenylethyne-linked dimers containing Mg- and Zn porphyrin units and trimers containing addnl. free-base unit)
IT Metalloporphyrins
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(magnesium; photoinduced energy transfer in diphenylethyne-linked

dimers containing Mg- and Zn porphyrin units and trimers containing addnl. free-base unit)

IT Electric switches
(optoelectronic; photoinduced energy transfer in diphenylethyne-linked dimers containing Mg- and Zn porphyrin units and trimers containing addnl. free-base unit in relation to)

IT Absorption spectra
Fluorescence
(photoinduced energy transfer in diphenylethyne-linked dimers containing Mg- and Zn porphyrin units and trimers containing addnl. free-base unit)

IT Porphyrins
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(photoinduced energy transfer in diphenylethyne-linked multiporphyrin arrays)

IT Optical absorption
(transient, decay kinetics; photoinduced energy transfer in diphenylethyne-linked dimers containing Mg- and Zn porphyrin units and trimers containing addnl. free-base unit)

IT Metalloporphyrins
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(zinc complexes; photoinduced energy transfer in diphenylethyne-linked dimers containing Mg- and Zn porphyrin units and trimers containing addnl. free-base unit)

IT 187342-24-1P, Ethyl 3-iodocinnamate 295800-87-2P, 3-Ethoxycarbonyl-4-(3-iodophenyl)pyrrole 295800-89-4P 295800-90-7P 295800-91-8P 295804-33-0P 295804-34-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in synthesis of porphyrin building blocks for multiporphyrin arrays)

IT 295800-88-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(in synthesis of porphyrin building blocks for multiporphyrin arrays)

IT **248243-80-3**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(photoinduced energy transfer in diphenylethyne-linked Mg- and Zn porphyrin dimers)

IT **295804-37-4P 295804-38-5P 295804-39-6P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(photoinduced energy transfer in diphenylethyne-linked Mg- and Zn porphyrin dimers)

IT **247103-35-1**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(photoinduced energy transfer in diphenylethyne-linked timers containing Mg- and Zn and free-base porphyrin units)

IT **295804-40-9P 295804-41-0P 295804-42-1P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(photoinduced energy transfer in diphenylethyne-linked timers containing Mg- and Zn and free-base porphyrin units)

IT 194035-39-7 247103-30-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of multiporphyrin arrays)

IT 295804-35-2P 295804-36-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

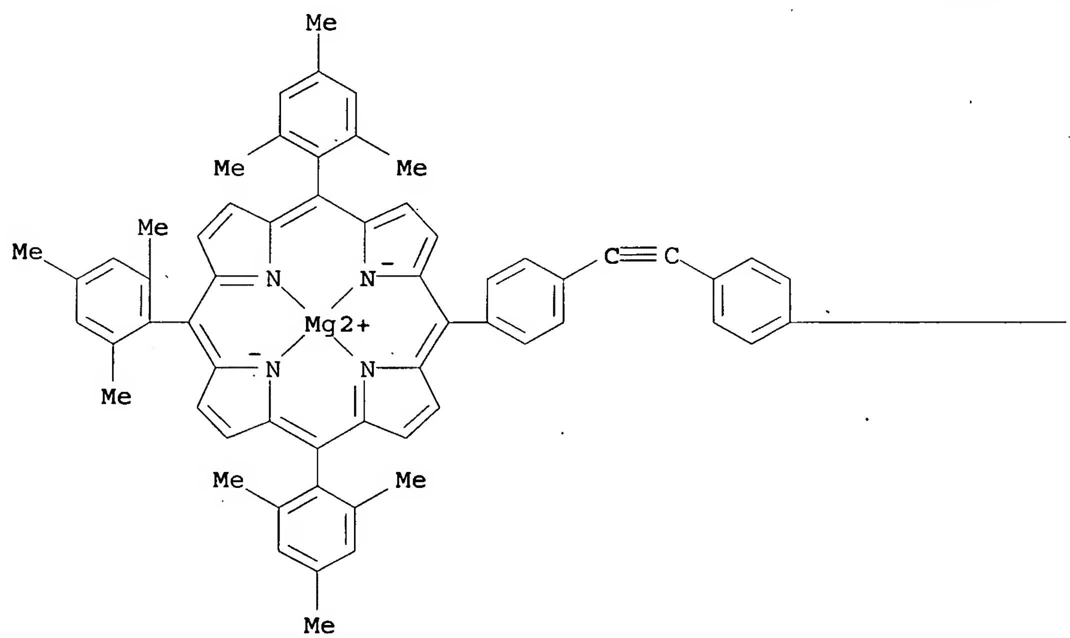
(synthesis of porphyrin building blocks for multiporphyrin arrays)

IT **248243-80-3**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(photoinduced energy transfer in diphenylethyne-linked Mg- and Zn porphyrin dimers)

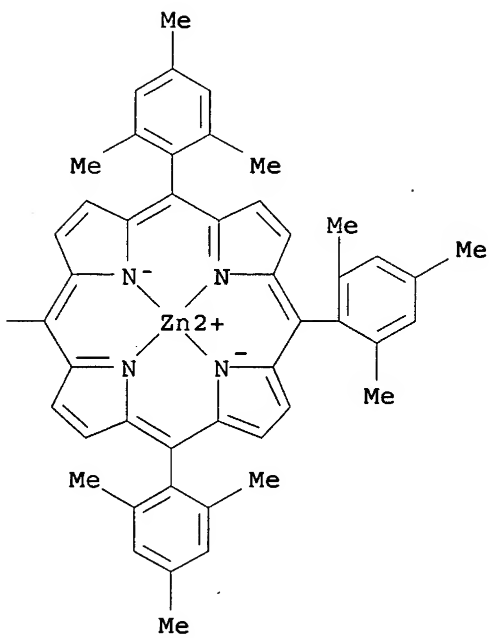
RN 248243-80-3 HCAPLUS

CN Magnesium, [μ-[[5,5'-(1,2-ethynediyldi-4,1-phenylene)bis[10,15,20-tris(2,4,6-trimethylphenyl)-21H,23H-porphinato-κN21,κN22,κN23,κN24]](4-)]](zinc)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 32 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:198530 HCAPLUS
DOCUMENT NUMBER: 132:340666
TITLE: Ultrafast Energy Relaxation Dynamics of Directly Linked Porphyrin Arrays
AUTHOR(S): Cho, Hyun Sun; Song, Nam Woong; Kim, Yong Hee; Jeoung, Sae Chae; Hahn, Sangjoon; Kim, Dongho; Kim, Seong Keun; Yoshida, Naoya; Osuka, Atsuhiro
CORPORATE SOURCE: National Creative Research Initiatives Center for Ultrafast Optical Characteristics Control and Spectroscopy Laboratory, Korea Research Institute of Standards and Science, Taejon, 305-600, S. Korea
SOURCE: Journal of Physical Chemistry A (**2000**), 104(15), 3287-3298
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A variety of porphyrin arrays connected together with different linkage were devised for possible applications to **mol.** optoelectronic **devices** such as wires, logic gates, and artificial light-harvesting arrays, etc. It was relatively well established that the light signal transmission in these mol. assemblies is based on exciton migration process, which possibly gives rise to the structural changes during the exciton delocalization process. Zn(II) 5,15-di(3,5-di-tert-butylphenyl)porphyrin (Z1), its directly meso, meso-linked porphyrin dimer (Z2), trimer (Z3), and tetramer (Z4) were synthesized with the goal to elucidate the relation between exciton migration and structural change upon photoexcitation. One of the most important factors in structural changes for these porphyrin arrays is mainly determined by the dihedral angle

between adjacent porphyrin moieties. For a systematic approach toward the study of the exciton coupling dynamics influenced by the relative orientation between neighboring porphyrin mols., various time-resolved spectroscopic techniques such as fluorescence decay and transient absorption measurements with different polarization in pump/probe beams were used. The steady-state excitation anisotropy spectra of Z2, Z3, and Z4 porphyrin arrays show that the photoexcitation of the high-energy exciton Soret band induces a large angle change between absorption and emission dipoles in contrast with the photoexcitation of the low-energy exciton split Soret and Q-bands. In the order of Z1, Z2, Z3, and Z4, their S1 states decay faster because of the increasing energy dissipation processes into a larger number of accessible states. The rotational diffusion rates become slower in the same order because the overall mol. shape is elongated along the long axis of the mol. arrays, which experiences a large displacement of solvent mols. in rotational diffusion motion. Ultrafast fluorescence decay measurements show that the S2 → S1 internal conversion process occurs in <1 ps in Z2, Z3, and Z4 due to the existence of exciton split band as a ladder-type deactivation channel, while this process is relatively slow in Z1 (.apprx.1.6 ps). Femtosecond transient absorption expts. with magic angle and different polarization in probe beam were performed to find the relation between energy relaxation and anisotropy dynamics upon photoexcitation. The internal conversion in Z2, Z3, and Z4 is accompanied by the incoherent energy hopping processes occurring in .ltorsim.200 fs judging from a large change in the anisotropy value in the transient absorption decay. The decay components with .apprx.8 ps time constant were observed in both fluorescence up-conversion and femtosecond transient absorption decays. These components are believed to arise from the conformational change in the excited states, because the dihedral angle distribution in these arrays is 90 ± 20° at ambient temperature from the AM1 calcn.

CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 22, 65, 76

ST fluorescence anisotropy decay internal conversion porphyrin dihedral angle

IT Optoelectronics
(fluorescence of porphyrins in relation to)

IT Optical anisotropy
(fluorescence; of porphyrins in relation to mol. structures)

IT Fluorescence
(of porphyrins in relation to band shifts and lifetimes)

IT Potential energy
(of porphyrins in relation to energy relaxation dynamics)

IT UV and visible spectra
(of porphyrins in relation to exciton coupling)

IT Fluorescence up-conversion
(of porphyrins in relation to fluorescence decay)

IT Internal conversion
(of porphyrins in relation to mol. structures measured by fluorescence decay)

IT Fluorescence decay
(of porphyrins in relation to structural changes)

IT Diffusion
(rotational; of porphyrins in relation to mol. structures)

IT Molecular structure-property relationship
(spectra; of porphyrins)

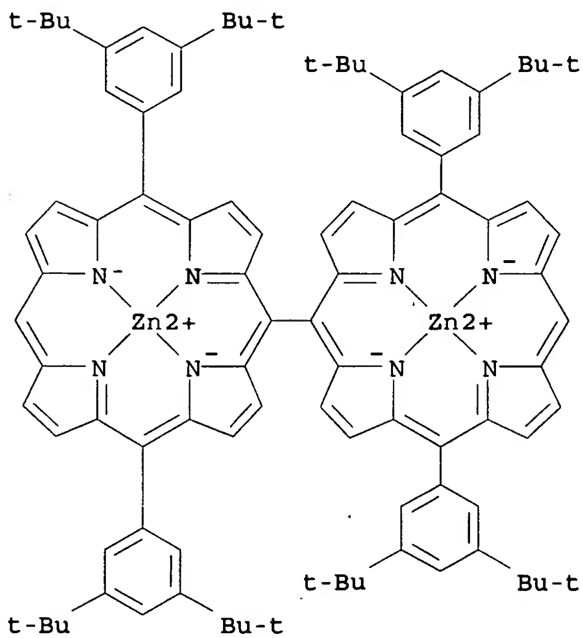
IT 187387-14-0
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(tultrafast energy relaxation dynamics of porphyrins in relation to conformational change)

IT **187387-16-2 187387-17-3 187387-19-5**
267418-48-4 267418-49-5 267418-50-8
267418-51-9 267418-52-0 267418-53-1
267418-54-2
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(ultrafast energy relaxation dynamics of porphyrins in relation to conformational change)

IT **187387-16-2**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(ultrafast energy relaxation dynamics of porphyrins in relation to conformational change)

RN 187387-16-2 HCAPLUS

CN Zinc, [μ-[10,10',20,20'-tetrakis[3,5-bis(1,1-dimethylethyl)phenyl]-5,5'-bi-21H,23H-porphinato(4-)-κN21,κN22,κN23,κN24:.kap pa.N21',κN22',κN23',κN24']]di- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 134 THERE ARE 134 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 33 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:165511 HCAPLUS
DOCUMENT NUMBER: 132:299419
TITLE: Space-resolved study of porphyrin rings: local optical properties and formation mechanism
AUTHOR(S): Vanoppen, Peter; Latterini, Loredana; Jeuris, Karin; Hofkens, Johan; De Schryver, Frans C.; Blossey, Ralf; Kerimo, Josef; Barbara, Paul F.; Rowan, Allen E.; Nolte, Roeland J. M.
CORPORATE SOURCE: Department of Chemistry, Katholieke Universiteit Leuven, Heverlee-Leuven, 3001, Belg.
SOURCE: Organic Mesoscopic Chemistry (**1999**), 75-87.

Editor(s): Masuhara, Hiroshi; De Schryver, Frans C.
Blackwell Science Ltd.: Oxford, UK.
CODEN: 68SAAI

DOCUMENT TYPE: Conference
LANGUAGE: English

AB The authors present details on the formation and characterization of the structures obtained through evaporation of solns. with porphyrin-based mols. and the proposal of a model for the ring formation mechanism. The films prepared using two different porphyrin derivs. were characterized using NSOM, CFM and AFM. An effect of the solute nature on the mol. organization of the ring assemblies has been observed using polarization imaging with NSOM. An exptl. study of the ring formation process by varying the sample preparation conditions was carried out with the aim of characterizing some of the factors affecting the ring growth mechanism. The effect of changes in **substrate** temperature, pressure and solvent evaporation rate on the ring formation process indicated that evaporation of the solvent is one of the main processes leading to the ring formation. Theor. arguments are presented to interpret the observations as a three-step process involving film rupture, contact line fluctuations and solvent-solute hydrodynamics.

CC 66-5 (Surface Chemistry and Colloids)
Section cross-reference(s): 22, **73**

ST porphyrin film morphol solvent evapn optical microscopy

IT Evaporation
(effect of **substrate** temperature, pressure and solvent evaporation rate on ring formation of in porphyrin thin films)

IT Films
Surface structure
(properties and formation mechanism of porphyrin rings studied by NSOM, CFM, and AFM)

IT Porphyrins
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(properties and formation mechanism of porphyrin rings studied by NSOM, CFM, and AFM)

IT **199739-23-6** 216973-27-2
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(properties and formation mechanism of porphyrin rings studied by NSOM, CFM, and AFM)

IT **199739-23-6**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(properties and formation mechanism of porphyrin rings studied by NSOM, CFM, and AFM)

RN 199739-23-6 HCAPLUS

CN Platinum, dichlorobis[5,10,15-tris[4-(hexadecyloxy)phenyl]-20-(4-pyridinyl-κN)-21H,23H-porphine]- (9CI) (CA INDEX NAME)

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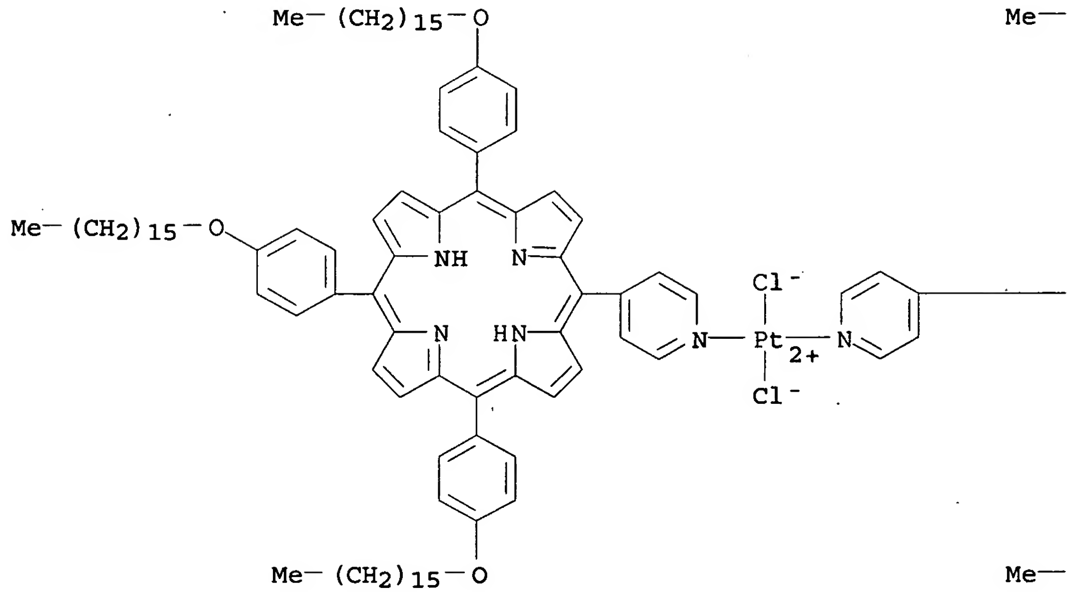

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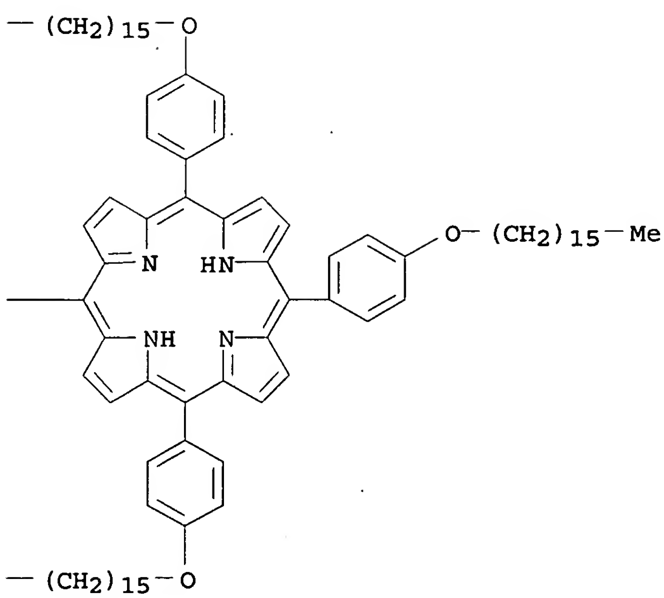


REFERENCE COUNT: 24   THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
                                    RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 34 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:369556 HCAPLUS
DOCUMENT NUMBER: 131:178866
TITLE: Synthesis of β-substituted porphyrin building
                            blocks and conversion to diphenylethyne-linked

porphyrin dimers

AUTHOR(S): Balasubramanian, Thiagarajan; Lindsey, Jonathan S.
CORPORATE SOURCE: Department of Chemistry, North Carolina State University, Raleigh, NC, 27695-8204, USA

SOURCE: Tetrahedron (**1999**), 55(22), 6771-6784
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A recent hypothesis concerning effects of orbital ordering on electronic communication (excited-state energy transfer, ground-state hole-hopping) in covalently linked porphyrin arrays prompted the development and application of methodol. for the synthesis of β-linked porphyrin dimers. Reaction of a β-substituted pyrrole with 2-hydroxymethylpyrrole led to the dipyrromethane bearing a single β-substituent and no meso- nor α-substituents. Condensation of the β-substituted dipyrromethane with an aldehyde and a meso-substituted dipyrromethane gave the desired β-substituted porphyrin building block, albeit in low yield. Four building blocks were prepared with a p-iodophenyl or p-ethynylphenyl group at one β-position, no substituent at the flanking meso-position, and mesityl or pentafluorophenyl groups at the three nonflanking meso-positions. The porphyrin building blocks were coupled via Pd-mediated reactions, affording diphenylethyne-linked dimers with the linker attached at β-positions. This approach provided access to zinc-free base porphyrin dimers and bis-zinc dimers bearing mesityl or pentafluorophenyl groups at the three nonlinking meso-positions. The availability of these dimers and monomeric benchmarks enabled a critical test of the orbital ordering hypothesis. This methodol. for preparing porphyrin building blocks bearing a lone, nonhindered β-substituent complements existing methods for preparing meso-substituted porphyrin building blocks. The ability to position the linker at the meso- or β-positions provides a desirable level of versatility for incorporating porphyrinic mols. with an a2u or a1u HOMO in various **mol. devices.**

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 26

ST zinc porphyrinato complex dimer prepn; porphyrin beta substituted dimer zinc prepn; metalloporphyrin zinc dimer beta substituted prepn

IT Porphyrins
RL: SPN (Synthetic preparation); PREP (Preparation)
(dimers; preparation of β-substituted porphyrins and zinc metalloporphyrins and β-linked zinc and zinc-free porphyrin dimers)

IT Porphyrins
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of β-substituted porphyrins and zinc metalloporphyrins and β-linked zinc and zinc-free porphyrin dimers)

IT Metalloporphyrins
RL: SPN (Synthetic preparation); PREP (Preparation)
(zinc complexes; preparation of β-substituted porphyrins and zinc metalloporphyrins and β-linked zinc and zinc-free porphyrin dimers)

IT 34633-08-4P 238760-82-2P 238760-84-4P 238760-86-6P 238760-88-8P 238760-90-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate product in preparation of β-substituted porphyrins and β-linked porphyrin dimers)

IT 226419-76-7P 226419-78-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and demetalation)

IT **226419-72-3P** **226419-74-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and metalation)

IT 226405-75-0P 226405-79-4P 226405-81-8P 226419-80-3P 226419-82-5P 238761-02-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction to give β-linked porphyrin dimers)

IT 226405-78-3P 238760-92-4P **238761-06-3P** **238761-08-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 487-68-3, Mesitaldehyde 653-37-2, Pentafluorobenzaldehyde 1066-54-2, Trimethylsilylacetylene 1071-46-1, Monoethyl malonate 15164-44-0, 4-Iodobenzaldehyde 36635-61-7, Tosylmethylisocyanide 86318-61-8, tert-Butyldimethylsilylacetylene 159152-14-4, 5-Mesityldipyrromethane 167482-91-9, 5-(Pentafluorophenyl)dipyrromethane 175689-33-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of β-substituted porphyrins and β-linked porphyrin dimers)

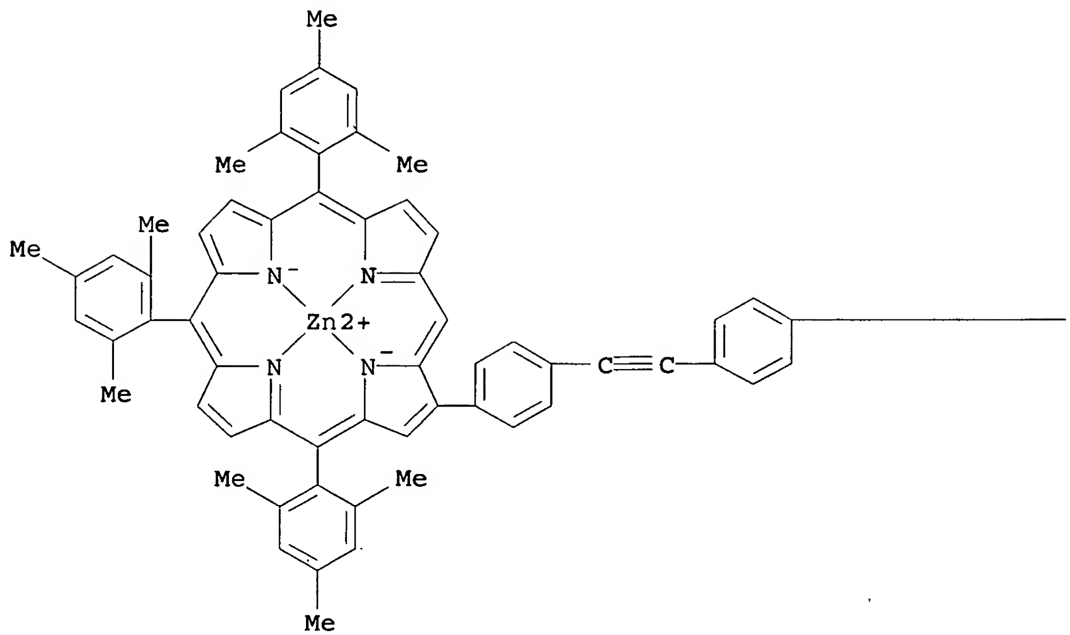
IT 25440-14-6P, meso-Tetrakis(pentafluorophenyl)porphyrin 238761-13-2P, 5,10,15-Tris(pentafluorophenyl)porphyrin 238761-14-3P 238761-15-4P
RL: BYP (Byproduct); PREP (Preparation)
(scrambled byproduct in preparation of β-substituted porphyrin)

IT **226419-72-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and metalation)

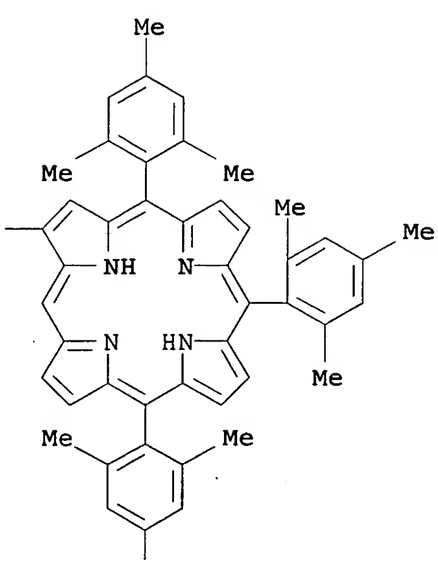
RN 226419-72-3 HCAPLUS

CN Zinc, [5,10,15-tris(2,4,6-trimethylphenyl)-2-[4-[[4-[5,10,15-tris(2,4,6-trimethylphenyl)-21H,23H-porphin-2-yl]phenyl]ethynyl]phenyl]-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-2)-
(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



PAGE 2-B

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REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 35 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:350782 HCAPLUS
DOCUMENT NUMBER: 130:359585
TITLE: Low pressure vapor phase deposition of organic thin films
INVENTOR(S): Forrest, Stephen R.; Burrows, Paul; Ban, Vladimir S.
PATENT ASSIGNEE(S): The Trustees of Princeton University, USA
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9925894	A1	19990527	WO 1998-US24424		19981116 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW					
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US 6337102	B1	20020108	US 1997-972156		19971117 <--
AU 9914124	A1	19990607	AU 1999-14124		19981116 <--
EP 1032722	A1	20000906	EP 1998-957997		19981116 <--
EP 1032722	B1	20041027			
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JP 2001523768	T2	20011127	JP 2000-521253		19981116 <--
TW 575699	B	20040211	TW 1998-87118943		19981117 <--
US 2001002279	A1	20010531	US 2000-736090		20001213 <--
US 2002155230	A1	20021024	US 2002-125400		20020419 <--
US 6558736	B2	20030506			
US 2004007178	A1	20040115	US 2003-427933		20030502 <--
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			US 2000-663143	B1	20000915 <--
			US 2000-736090	A1	20001213 <--
			US 2002-125400	A3	20020419 <--

AB Methods for preparing organic thin films on **substrates** are described which entail providing a plurality of organic precursors in the vapor phase, and reacting the plurality of organic precursors at a pressure below atmospheric pressure to produce a film on the **substrate**. The methods may be applied to the production of organic light-emitting **devices**. Apparatus for carrying out the methods is described which comprises a reaction chamber; means for heating the reaction chamber; means for introducing vapors of organic precursor materials into the reaction chamber; and means for reducing

the pressure in the reaction chamber to below atmospheric pressure. Apparatus is also
described which includes a plurality of vacuum chambers and a conveyor for moving **substrates** between them. Films, including light-emitting and nonlinear optical material films, formed by the methods are also claimed.

IC ICM C23C016-00
ICS H01J001-62

CC 75-1 (Crystallography and Liquid Crystals)
Section cross-reference(s): **73**, 76

ST low pressure org vapor deposition app; electroluminescent **device** fabrication low pressure org vapor deposition; nonlinear optical film low pressure org vapor deposition; light emitting film low pressure org vapor deposition

IT Vapor deposition process
(chemical; methods for low pressure vapor phase deposition of organic thin films and deposition apparatus and films produced by the methods)

IT Phosphors
(electroluminescent; methods and apparatus for low pressure vapor phase deposition of organic)

IT Nonlinear optical materials
(methods and apparatus for low pressure vapor phase deposition of organic)

IT Electroluminescent **devices**
Electroluminescent **devices**
Semiconductor **device** fabrication
(methods and. apparatus for low pressure vapor phase deposition of organic thin
films for)

IT Films
Vapor deposition apparatus
(methods for low pressure vapor phase deposition of organic thin films and deposition apparatus and films produced by the methods)

IT 7439-90-9, Krypton, processes 7440-01-9, Neon, processes 7440-37-1, Argon, processes 7440-59-7, Helium, processes 7440-63-3, Xenon, processes 7727-37-9, Nitrogen, processes
RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(carrier gas; methods for low pressure vapor phase deposition of organic thin films and deposition apparatus and films produced by the methods)

IT 66-27-3, Methyl methanesulfonate 80-48-8, Methyl tosylate 333-27-7, Methyl trifluoromethanesulfonate 431-47-0, Methyl trifluoroacetate 889-36-1, 4'-Dimethylamino-4-stilbazole 959-81-9, 4'-Dimethylamino-N-methyl-4-stilbazolium iodide 1518-16-7 26908-82-7, Acetyl p-toluenesulfonate 29519-52-6, 4'-Dimethylamino-4-ethylstilbazolium iodide 31366-25-3 113657-21-9 224769-09-9, 4'-Dimethylamino-4-methylstilbazolium thiophenoxide 224769-10-2, 4'-Dimethylamino-4-ethylstilbazolium hydroxide
RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(film precursor; methods for low pressure vapor phase deposition of organic thin films and deposition apparatus and films produced by the
methods)

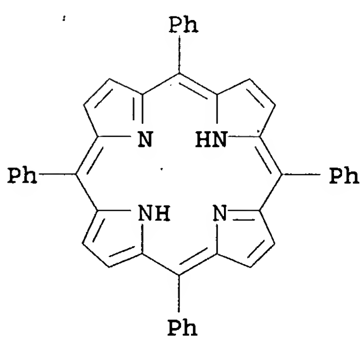
IT **917-23-7P**, 5,10,15,20-Tetraphenyl-21H,23H-porphine 2085-33-8P, Tris(8-hydroxyquinolinato)aluminum 51325-91-8P, 4-(Dicyanomethylene)-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran 65181-78-4P, N,N'-Diphenyl-N,N'-bis(3-methylphenyl)-1,1'-biphenyl-4,4'-diamine 123847-85-8P 124729-98-2P, MTDATA 224785-36-8P
RL: IMF (Industrial manufacture); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); TEM (Technical or engineered

material use); **PREP (Preparation)**; PROC (Process); USES (Uses)
(methods for low pressure vapor phase deposition of organic thin films and deposition apparatus and films produced by the methods)

IT 24235-06-1P, 4'-Dimethylamino-N-methyl-4-stilbazolium tosylate
40210-84-2P 113657-23-1P, 4'-Methoxy-4-methylstilbazolium tosylate
148624-15-1P, 4'-Dimethylamino-4-methylstilbazolium methanesulfonate
224769-11-3P, 4'-Dimethylamino-4-methylstilbazolium trifluoromethanesulfonate 224769-13-5P 224769-14-6P,
4'-Dimethylamino-4-methylstilbazolium trifluoroacetate
RL: IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); PREP (Preparation); PROC (Process); USES (Uses)
(methods for low pressure vapor phase deposition of organic thin films and deposition apparatus and films produced by the methods)

IT **917-23-7P**, 5,10,15,20-Tetraphenyl-21H,23H-porphine
RL: IMF (Industrial manufacture); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); **PREP (Preparation)**; PROC (Process); USES (Uses)
(methods for low pressure vapor phase deposition of organic thin films and deposition apparatus and films produced by the methods)

RN 917-23-7 HCAPLUS
CN 21H,23H-Porphine, 5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 36 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:245313 HCAPLUS
DOCUMENT NUMBER: 131:73471
TITLE: Ring Formation in Evaporating Porphyrin Derivative Solutions
AUTHOR(S): Latterini, L.; Blossey, R.; Hofkens, J.; Vanoppen, P.; De Schryver, F. C.; Rowan, A. E.; Nolte, R. J. M.
CORPORATE SOURCE: Department of Chemistry, Katholieke Universiteit Leuven, Louvain, B-3001, Belg.
SOURCE: Langmuir (**1999**), 15(10), 3582-3588
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The formation of micrometer-size, ring-shaped structures is studied in evaporating solns. of porphyrin-based mols. on glass. Solute concentration, solution and **substrate** temperature, vapor pressure, and solvent are varied. The mol. arrangements on the **substrate** are monitored by confocal

fluorescence microscopy (CFM), atomic force microscopy (AFM), and near-field scanning optical microscopy (NSOM). From experiment, a nonequil. morphol. diagram for the observed structures is deduced as a function of solute concentration
and evaporation time. The mechanisms involved in ring formation are discussed on the basis of solvent and solute dynamics.

CC 26-7 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): **36**, **66**, **73**

ST platinum porphyrin wheel aggregate chloroform; ring assembly glass evapn

IT Glass **substrates**
Molecular association
(formation mechanism of ring shaped mol. aggregates in evaporating porphyrin derivative solns. studied by CFM, AFM, and NSOM)

IT Metalloporphyrins
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(platinum; formation mechanism of ring shaped mol. aggregates in evaporating porphyrin derivative solns. studied by CFM, AFM, and NSOM)

IT **199739-23-6**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(formation mechanism of ring shaped mol. aggregates in evaporating porphyrin derivative solns. studied by CFM, AFM, and NSOM)

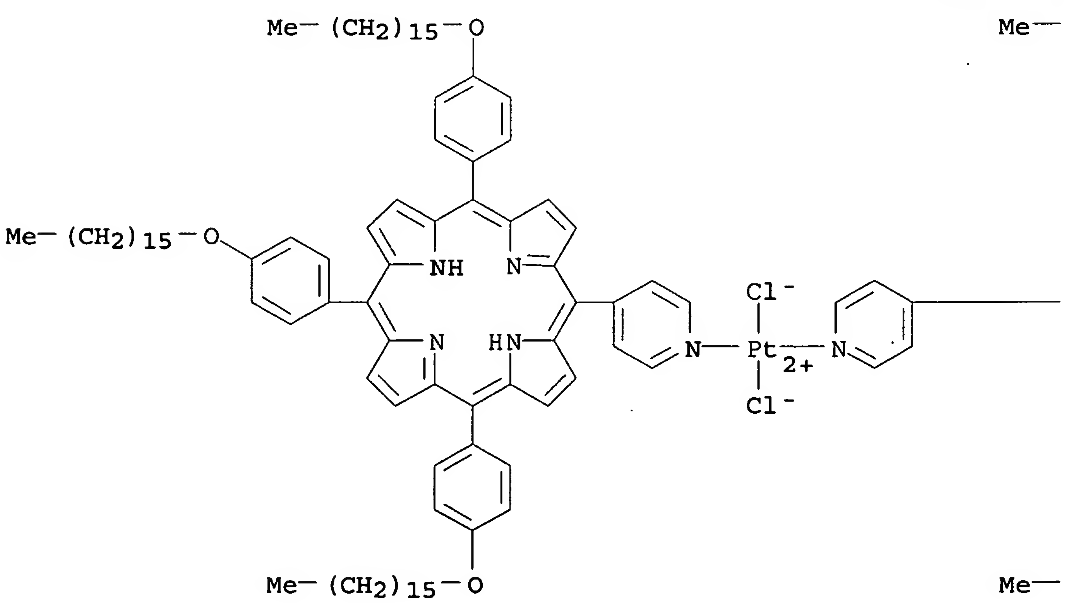
IT 67-66-3, Chloroform, properties 120-82-1, 1,2,4-Trichlorobenzene
RL: PRP (Properties)
(formation mechanism of ring shaped mol. aggregates in evaporating porphyrin derivative solns. studied by CFM, AFM, and NSOM)

IT **199739-23-6**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(formation mechanism of ring shaped mol. aggregates in evaporating porphyrin derivative solns. studied by CFM, AFM, and NSOM)

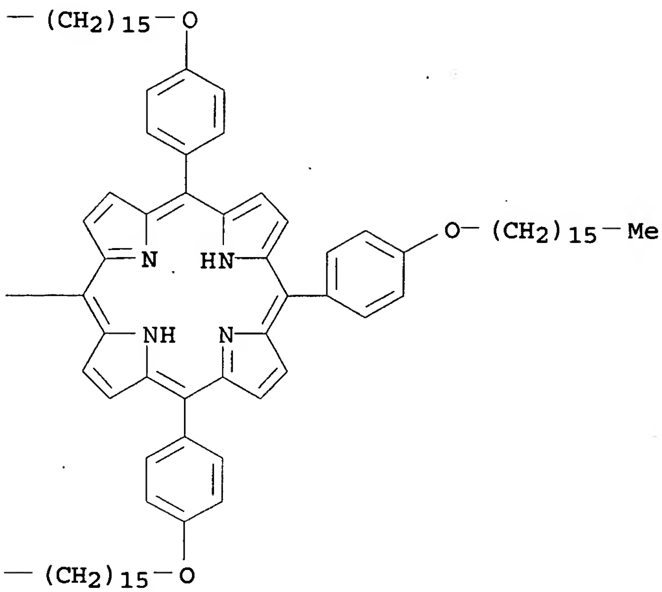
RN 199739-23-6 HCAPLUS

CN Platinum, dichlorobis[5,10,15-tris[4-(hexadecyloxy)phenyl]-20-(4-pyridinyl-κN)-21H,23H-porphine]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1999:234511 HCAPLUS
DOCUMENT NUMBER: 131:25637
TITLE: Interplay of Orbital Tuning and Linker Location in Controlling Electronic Communication in Porphyrin Arrays
AUTHOR(S): Yang, Sung Ik; Seth, Jyoti; Balasubramanian, Thiagarajan; Kim, Dongho; Lindsey, Jonathan S.; Holten, Dewey; Bocian, David F.
CORPORATE SOURCE: Departments of Chemistry, North Carolina State University, Raleigh, NC, 27695-8204, USA
SOURCE: Journal of the American Chemical Society (**1999**), 121(16), 4008-4018
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The β-diphenylethyne-linked porphyrin dimers ZnFbU-β (nonlinking meso-mesityl substituents) and F30ZnFbU-β (nonlinking meso-pentafluorophenyl substituents) and their bis-Zn analogs have been examined by static spectroscopic (absorption, fluorescence, ESR), time-resolved spectroscopic (absorption, fluorescence), and electrochem. (cyclic and square-wave voltammetry, coulometry) methods. The β-linked dimers were examined to test the hypothesis that the nature of the porphyrin HOMO (a1u vs. a2u) in concert with the position of the linker (β-pyrrole or meso carbon) mediates electronic communication (excited-state energy transfer, ground-state hole-hopping). The major findings are as follows: (1) The rate of energy transfer is (56 ps)-1 for ZnFbU-β and (24 ps)-1 for F30ZnFbU-β; (2) The rate of

hole/electron hopping in the monooxidized bis-Zn complex [F30Zn2U-β]+ is in the fast-exchange limit and is at least comparable to that for [Zn2U-β]+. These findings indicate that the presence of pentafluorophenyl groups causes enhancement of electronic communication in the β-linked dimers but attenuation in the meso-linked dimers. These opposite effects in the β- vs. meso-linked dimers are explained by the fact that both pentafluorophenyl-substituted dimers have a1u HOMOs, which exhibit significant β-pyrrole electron d., whereas both mesityl-substituted dimers have a2u HOMOs, which exhibit large meso-carbon d. Thus, the combination of an a1u HOMO with a β-linker or an a2u HOMO with a meso linker results in optimal electronic communication. Collectively, these results demonstrate that the nature of the frontier orbitals and position of connection of a covalent linker (in addition to distance, orientation, and energetics) must be considered in the design architecture of **mol.** photonic **devices.**

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 26, 76, 78

ST beta linked porphyrin dimer electronic communication photoinduced energy transfer; HOMO meso linked porphyrin dimer design **mol** photonic **device**

IT Porphyrins
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(dimers; enhancement of electronic communication in β-linked dimers and attenuation in meso-linked dimers for design of **mol** . photonic **device**)

IT Molecular structure-property relationship
(electronic structure; enhancement of electronic communication in β-linked dimers and attenuation in meso-linked dimers for design of **mol.** photonic **device**)

IT Conformation
Fluorescence
HOMO (molecular orbital)
Hopping conductivity
Photoinduced energy transfer
Photonics
(enhancement of electronic communication in β-linked dimers and attenuation in meso-linked dimers for design of **mol.** photonic **device**)

IT Electron transfer kinetics
(intramol., photochem.; enhancement of electronic communication in β-linked dimers and attenuation in meso-linked dimers for design of **mol.** photonic **device**)

IT **226419-72-3 226419-74-5**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(enhancement of electronic communication in β-linked dimers and attenuation in meso-linked dimers for design of **mol.** photonic **device**)

IT 226405-75-0 226405-78-3 226405-79-4 226405-81-8 226419-76-7 226419-78-9 226419-80-3 226419-82-5
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(reference; enhancement of electronic communication in β-linked dimers and attenuation in meso-linked dimers for design of **mol.** photonic **device**)

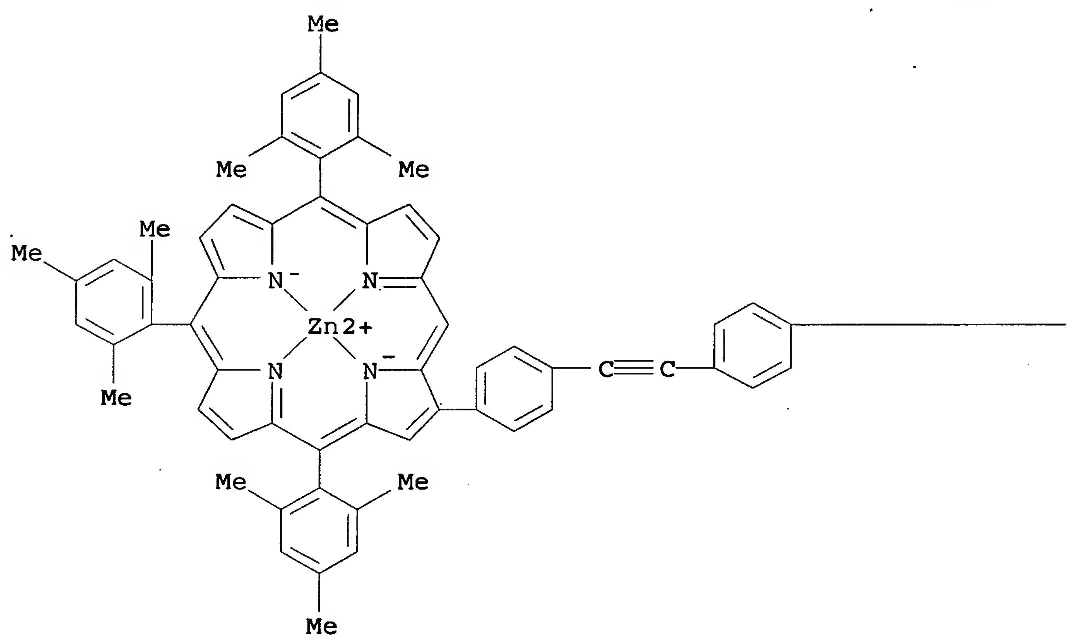
IT **226419-72-3**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(enhancement of electronic communication in β-linked dimers and attenuation in meso-linked dimers for design of **mol.** photonic **device**)

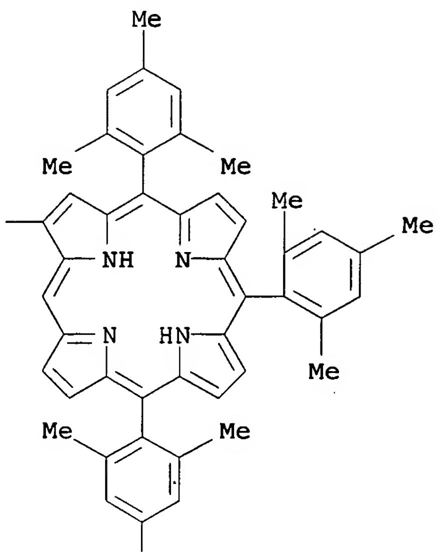
RN 226419-72-3 HCAPLUS

CN Zinc, [5,10,15-tris(2,4,6-trimethylphenyl)-2-[4-[[4-[5,10,15-tris(2,4,6-trimethylphenyl)-21H,23H-porphin-2-yl]phenyl]ethynyl]phenyl]-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-2)-
(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



PAGE 2-B

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 38 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:94268 HCAPLUS
DOCUMENT NUMBER: 130:278459
TITLE: Substrates for rapid delivery of electrons and holes to buried active sites in proteins
AUTHOR(S): Wilker, Jonathan J.; Dmochowski, Ivan J.; Dawson, John H.; Winkler, Jay R.; Gray, Harry B.
CORPORATE SOURCE: Beckman Institute, California Institute of Technology, Pasadena, CA, 91125, USA
SOURCE: Angewandte Chemie, International Edition (**1999**), 38(1/2), 90-92
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors developed a powerful photochem. method for the delivery of electrons and holes to buried redox sites. By tethering a Ru photosensitizer to a protein substrate, they have succeeded in reducing the P 450 heme much more rapidly than previously possible and they have generated a previously unobserved oxidized state of the enzyme. The photosensitizer [Ru(bpy)3]2+ (bpy= 2,2'-bipyridine) is linked through a hydrocarbon chain to a species with high affinity for the P 450 heme

pocket: imidazole, adamantane, or ethylbenzene. Imidazole ligates the heme iron center directly, whereas adamantane and ethylbenzene bind strongly to the hydrophobic cavity of the active site.

CC 7-3 (Enzymes)

ST ruthenium photosensitizer cytochrome P450 redn

IT Photoinduced electron transfer
(Ru photosensitizer tethered to substrate for reducing cytochrome P 450 heme)

IT Enzyme **functional** sites
(active; Ru **photosensitizer** tethered to substrate for reducing cytochrome P 450 heme)

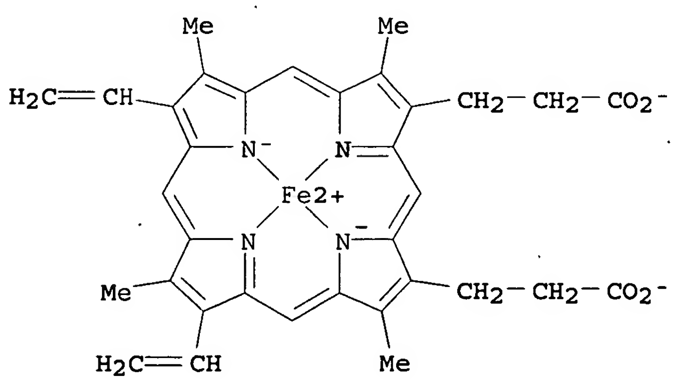
IT 9035-51-2, Cytochrome P 450, biological studies
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(Ru photosensitizer tethered to substrate for reducing cytochrome P 450 heme)

IT **14875-96-8**, Heme 222719-03-1 222719-04-2 222719-05-3
RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(Ru photosensitizer tethered to **substrate** for reducing cytochrome P 450 heme)

IT **14875-96-8**, Heme
RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(Ru photosensitizer tethered to **substrate** for reducing cytochrome P 450 heme)

RN 14875-96-8 HCAPLUS

CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-κN21,κN22,κN23,κN24]-, dihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)



●2 H^+

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 39 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:568315 HCAPLUS

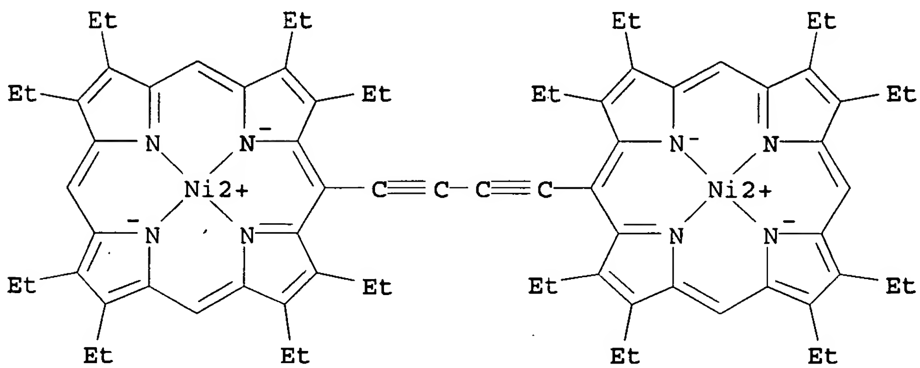
DOCUMENT NUMBER: 129:350267
TITLE: Gas-sensing properties of porphyrin dimer Langmuir-Blodgett films
AUTHOR(S): Arnold, D. P.; Manno, D.; Micocci, G.; Serra, A.; Tepore, A.; Valli, L.
CORPORATE SOURCE: Centre for Instrumental and Developmental Chemistry (C.I.D.C.), Queensland University of Technology, Brisbane, Australia
SOURCE: Thin Solid Films (**1998**), 327-329, 341-344
CODEN: THSFAP; ISSN: 0040-6090
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Langmuir-Blodgett films of a 1:4 mixture of meso, meso'-buta-1,3-diyne-bridged Ni(II) octaethylporphyrin dimer and arachidic acid were deposited onto various **substrates.** The isotherm at the air/water interface and absorbance measurements using polarized light are consistent with a planar statistical orientation of the porphyrin dimers which are probably prone onto the arachidic acid tails. The presence in the dimer of the acetylenic linking group gave a large and highly conjugated mol. structure; this suggested the use of the films in gas sensing apparatus Elec. characterization in controlled atmospheric and with the simultaneous presence of interfering gaseous species, such as EtOH, NH3, and CO, suggest that this porphyrin dimer is a promising selective NO gas sensing material.
CC 79-3 (Inorganic Analytical Chemistry)
Section cross-reference(s): 26, 59, 66, **73**
ST gas sensing porphyrin dimer Langmuir Blodgett; sensor porphyrin dimer Langmuir Blodgett film
IT Dichroism
Molecular orientation
(average mol. orientation of porphyrin dimer Langmuir-Blodgett films based on absorbance measurements with polarized light and linear dichroism method)
IT Gas analysis
Gas sensors
Langmuir-Blodgett films
(nitric oxide determination by gas sensor based on Langmuir-Blodgett films of meso, meso'-buta-1,3-diyne-bridged Ni(II) octaethylporphyrin dimer and arachidic acid)
IT Optical dispersion
(optical dispersion curves of Langmuir-Blodgett films of mixture of meso, meso'-buta-1,3-diyne-bridged Ni(II) octaethylporphyrin dimer and arachidic acid)
IT Surface pressure-area isotherms
(surface pressure-area isotherm of 1:4 mixture of meso, meso'-buta-1,3-diyne-bridged Ni(II) octaethylporphyrin dimer and arachidic acid)
IT 10102-43-9, Nitric oxide, analysis
RL: ANT (Analyte); ANST (Analytical study)
(nitric oxide determination by gas sensor based on Langmuir-Blodgett films of meso, meso'-buta-1,3-diyne-bridged Ni(II) octaethylporphyrin dimer and arachidic acid)
IT 506-30-9, Arachidic acid **67168-57-4**
RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)
(nitric oxide determination by gas sensor based on Langmuir-Blodgett films of

meso, meso'-buta-1,3-diyne-bridged Ni(II) octaethylporphyrin dimer and arachidic acid)

IT **67168-57-4**
RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)
(nitric oxide determination by gas sensor based on Langmuir-Blodgett films of
meso, meso'-buta-1,3-diyne-bridged Ni(II) octaethylporphyrin dimer and arachidic acid)

RN 67168-57-4 HCAPLUS

CN Nickel, [μ-[[5,5'-(1,3-butadiyne-1,4-diyl)bis[2,3,7,8,12,13,17,18-octaethyl-21H,23H-porphinato-κN21,κN22,κN23,κN24]](4-)]]di- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 40 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:496362 HCAPLUS
DOCUMENT NUMBER: 129:183363
TITLE: Modular Synthesis of Benzene-Centered Porphyrin Trimers and a Dendritic Porphyrin Hexamer
AUTHOR(S): Mongin, Olivier; Papamicael, Cyril; Hoyler, Nicolas; Gossauer, Albert
CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet, Fribourg, CH-1700, Switz.
SOURCE: Journal of Organic Chemistry (**1998**), 63(16), 5568-5580
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Rigid, star-shaped D3-sym. arrays were synthesized in which three porphyrin macrocycles are attached to the 1, 3, and 5 positions each of a benzene core through linkers consisting of collinear repetitive phenylethynyl units. Using the same methodol., a dendritic porphyrin hexamer having an external diameter of .apprx.10 nm was also obtained. By successive substitution of the three benzene positions, both a porphyrin trimer, the three linkers of which are of different length, and a starlike porphyrin, in which the complexed metal ions are different from each other, were synthesized. The latter is the 1st example of a prochiral arrangement of metal ions in a D3-sym. ligand. To investigate their capability of forming ordered self-assembled monolayers on gold **substrates**, some of the porphyrin trimers and the dendritic

porphyrin hexamer described in this work bear meta-thioanisole units at the apical positions. Analogously to similar multiporphyrin systems described in the literature, in which, however, the chromophores were arranged collinearly, the interaction between the chromophores of the multiporphyrin arrays described in this work is negligible, in the ground state, while effective energy transfer takes place in the singlet excited state.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 26, **73**, 74

ST metalloporphyrin trimer dendritic hexamer prepn; zinc porphyrinato homometallic heterometallic trimer prepn; transition metal porphyrinato trinuclear hexanuclear prepn

IT Energy transfer
(in excited state of zinc-nickel-copper heterometallic trimeric porphyrinato complexes)

IT Fluorescence
(of transition metal porphyrinato trimeric homo- and heterometallic and zinc dendritic hexameric complexes)

IT Transition metal complexes
Transition metal complexes
RL: SPN (Synthetic preparation); PREP (Preparation)
(porphyrin; preparation of transition metal porphyrinato trimeric homo- and heterometallic and zinc dendritic hexameric complexes)

IT Metalloporphyrins
Metalloporphyrins
RL: SPN (Synthetic preparation); PREP (Preparation)
(transition metal; preparation of transition metal porphyrinato trimeric homo- and heterometallic and zinc dendritic hexameric complexes)

IT 210907-47-4P
RL: BYP (Byproduct); PREP (Preparation)
(byproduct in preparation of mono-(methylthiophenyl)ethynyl analog)

IT 626-44-8, 1,3,5-Triiodobenzene 1066-54-2, (Trimethylsilyl)ethyne 33733-73-2, 1-Bromo-3-(methylthio)benzene 67973-34-6, 4,4'-Diiodotolane 159152-18-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of transition metal porphyrinato trimeric and zinc dendritic hexameric complexes)

IT 7567-63-7P, 1,3,5-Triethynylbenzene 18772-58-2P, 1,3,5-Tris(trimethylsilylethynyl)benzene 130416-73-8P 210905-25-2P 210905-68-3P 210905-75-2P 210905-79-6P 210905-86-5P 210905-93-4P 210905-99-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of transition metal porphyrinato trimeric and zinc dendritic hexameric complexes)

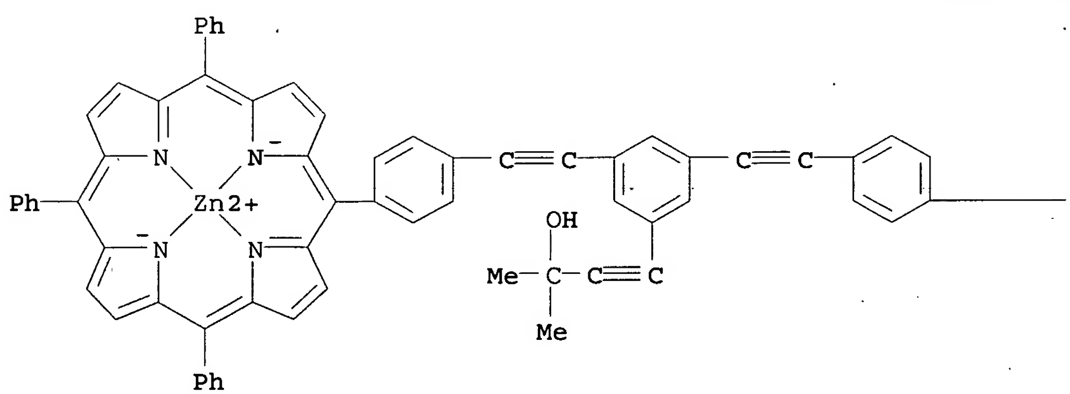
IT 115-19-5, 2-Methyl-3-butyn-2-ol 89343-06-6, (Triisopropylsilyl)ethyne 133513-05-0 134856-57-8 134856-58-9 159901-45-8 177991-06-9 191094-09-4 191094-14-1 191094-15-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of transition metal porphyrinato trimeric complexes)

IT 155064-31-6P 169231-40-7P 176977-35-8P 176977-37-0P 210905-13-8P 210905-19-4P 210905-30-9P 210905-41-2P 210906-07-3P 210906-75-5P 210906-81-3P 210906-88-0P 210906-95-9P 210907-01-0P **210907-07-6P** **210907-12-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of transition metal porphyrinato trimeric complexes)

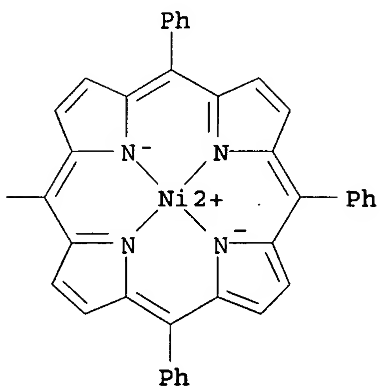
IT **210907-28-1P** **210907-32-7P** **210907-35-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for preparation of zinc porphyrinato dendritic hexameric complex)
IT 211301-38-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(for preparation of zinc porphyrinato dendritic hexameric complex)
IT 210906-43-7P **210906-55-1P 210906-61-9P**
210907-24-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and fluorescence quantum yield)
IT 210906-13-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction to remove silyl group)
IT 210906-19-7P **210906-49-3P 210906-69-7P** 211301-31-4P
211301-33-6P 211301-35-8P 211301-37-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **210907-16-7P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, fluorescence quantum yield and complexation with copper)
IT **210907-20-3P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, fluorescence quantum yield and zinc demetalation)
IT **210907-07-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of transition metal porphyrinato trimeric complexes)
RN 210907-07-6 HCAPLUS
CN Nickel, [μ-[4-[3,5-bis[[4-(10,15,20-triphenyl-21H,23H-porphin-5-yl-κN21,κN22,κN23,κN24)phenyl]ethynyl]phenyl]-2-methyl-3-butyn-2-olato(4-)]](zinc)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 41 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:269805 HCAPLUS
DOCUMENT NUMBER: 129:10133
TITLE: Energy-Transfer Modeling for the Rational Design of Multiporphyrin Light-Harvesting Arrays
AUTHOR(S): Van Patten, P. Gregory; Shreve, Andrew P.; Lindsey, Jonathan S.; Donohoe, Robert J.
CORPORATE SOURCE: Biochemistry and Biotechnology Group, Los Alamos National Laboratory, Los Alamos, NM, 87545, USA
SOURCE: Journal of Physical Chemistry B (**1998**), 102(21), 4209-4216
CODEN: JPCBFK; ISSN: 1089-5647
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Excited-state energy migration among a collection of pigments forms the basis for natural light-harvesting processes and synthetic **mol.** photonic **devices.** The rational design of efficient energy-transfer devices requires the ability to analyze the expected performance characteristics of target mol. architectures comprised of various pigments. A general tool is presented for modeling the kinetics of energy migration in weakly coupled multipigment arrays. A matrix-formulated eigenvalue/eigenvector approach was implemented, using empirical data from a small set of prototypical mols., to predict the quantum efficiency (QE) of energy migration in a variety of arrays as a function of rate, competitive processes, and architecture. Trends in the results point to useful design strategies including the following: (1) The QE for energy transfer to a terminal acceptor upon random excitation within a linear array of isoenergetic pigments decreases rapidly as the length of the array is increased. (2) Increasing the rate of transfer and/or the lifetime of the competitive deactivation processes significantly improves QE. (3) Qual. similar results are obtained in simulations of linear mol. photonic wires in which excitation and trapping occur at opposite ends of the array. (4) Branched and cyclic array architectures exhibit higher QEs than linear architectures with equal nos. of pigments. (5) Dramatic improvements in QE are achieved when energy transfer is directed by a progressive downward cascade in excited-state energy. (6) The most effective light-harvesting architectures are those where isolated pools of donors each have independent paths directly to the

terminal acceptor. Collectively, these results provide valuable insight into the types of mol. designs that are expected to exhibit high efficiency in overall energy transfer.

CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

ST energy transfer model multiporphyrin light harvesting

IT Light
(energy-transfer modeling for rational design of multiporphyrin arrays harvesting)

IT Electron acceptors
Electron donors
Excited state
Trapping
(energy-transfer modeling for rational design of multiporphyrin light-harvesting arrays in relation to)

IT Energy transfer
(modeling for rational design of multiporphyrin light-harvesting arrays)

IT Wires
(photonic; energy-transfer modeling for rational design of multiporphyrin light-harvesting arrays in relation to)

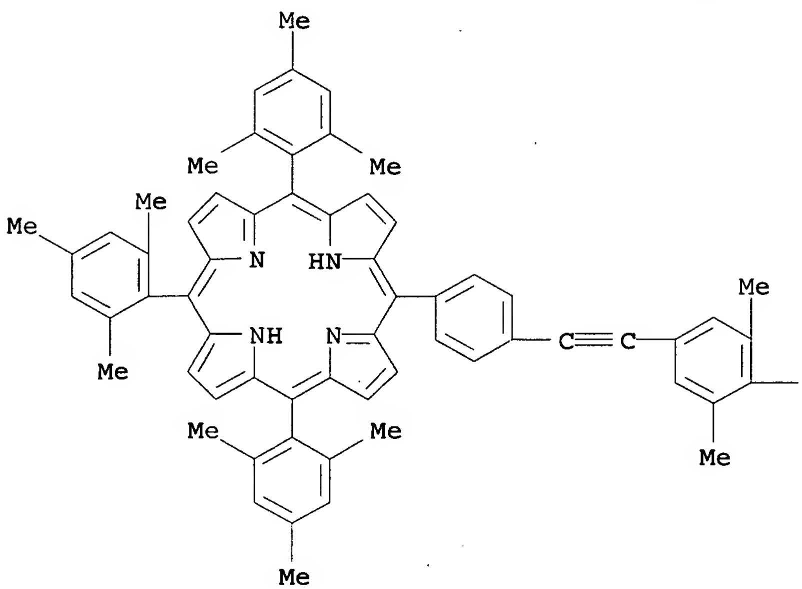
IT 500-77-6, 21H,23H-Porphyrazine 574-93-6, Phthalocyanine 917-23-7, Tetraphenylporphyrin 1661-03-6, Magnesium phthalocyanine 2042-48-0 2669-65-0 2683-82-1, Octaethylporphyrin 5143-18-0 14074-80-7 14320-04-8 14586-52-8 14640-21-2 14839-32-8 17632-18-7 22862-60-8 23627-89-6 27341-05-5 50795-70-5 57511-57-6 109122-74-9 144728-67-6D, derivs. **184154-24-3** 188532-35-6 188532-37-8 **207398-27-4** 207398-28-5 207464-23-1D, partially metalated derivs.
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(energy-transfer modeling for rational design of multiporphyrin light-harvesting arrays)

IT **184154-24-3**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(energy-transfer modeling for rational design of multiporphyrin light-harvesting arrays)

RN 184154-24-3 HCAPLUS

CN Zinc, [μ-[5-[2,6-dimethyl-4-[[4-[10,15,20-tris(2,4,6-trimethylphenyl)-21H,23H-porphin-5-yl]phenyl]ethynyl]phenyl]-10,20-bis(2,4,6-trimethylphenyl)-15-[4-[[4-[10,15,20-tris(2,4,6-trimethylphenyl)-21H,23H-porphin-5-yl-κN21,κN22,κN23,κN24]phenyl]ethynyl]ph
enyl]-21H,23H-porphinato(4-)-κN21,κN22,κN23,κN24]]
di- (9CI) (CA INDEX NAME)

PAGE 1-A



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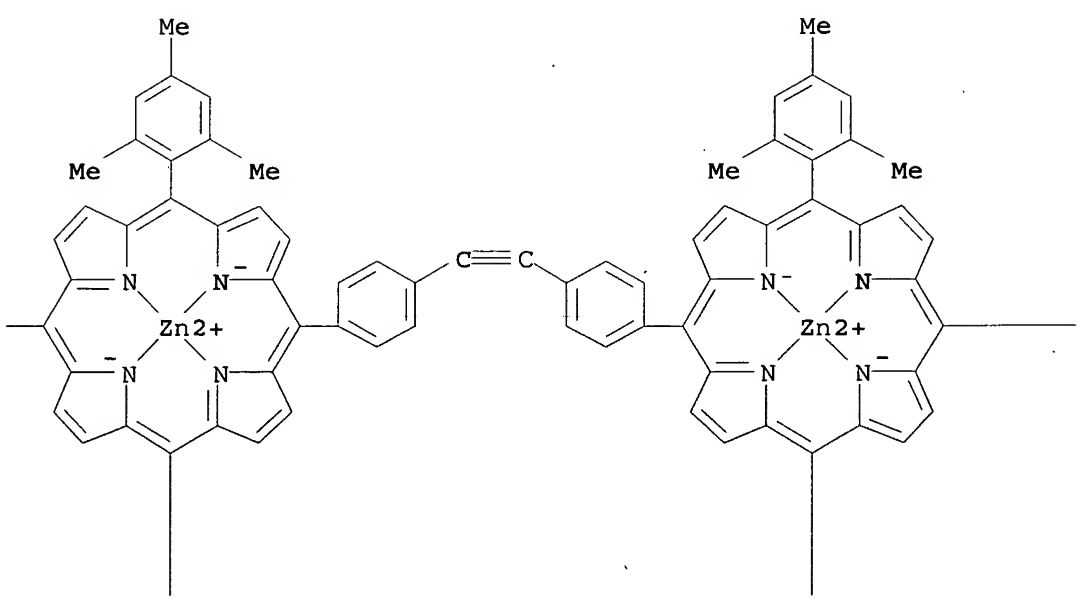
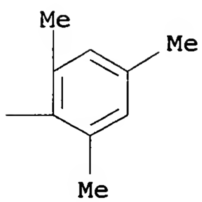
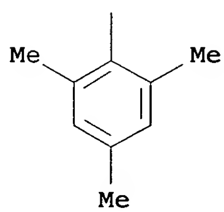
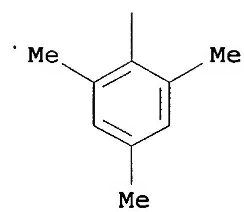


PAGE 1-C



PAGE 2-B





REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 42 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:740791 HCAPLUS
DOCUMENT NUMBER: 128:29650
TITLE: Effects of Orbital Ordering on Electronic Communication in Multiporphyrin Arrays
AUTHOR(S): Strachan, Jon-Paul; Gentemann, Steve; Seth, Jyoti; Kalsbeck, William A.; Lindsey, Jonathan S.; Holten, Dewey; Bocian, David F.
CORPORATE SOURCE: Departments of Chemistry, North Carolina State University, Raleigh, NC, 27695-8204, USA
SOURCE: Journal of the American Chemical Society (**1997**), 119(46), 11191-11201
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The rational design of **mol.** photonic **devices** requires a thorough understanding of all factors affecting electronic communication among the various constituents. To explore how electronic factors mediate both excited- and ground-state electronic communication in multiporphyrin arrays, the authors have conducted a detailed static spectroscopic (absorption, fluorescence, resonance Raman, ESR), time-resolved spectroscopic (absorption, fluorescence), and electrochem. (cyclic and square-wave voltammetry, coulometry) study of tetraarylporphyrin dimers.

The complexes studied include both Zn-free base (ZnFb) and bis-Zn dimers in which the porphyrin constituents are linked via diphenylethyne groups at the meso positions. Comparison of dimeric arrays containing pentafluorophenyl groups at all nonlinking meso positions (F30ZnFbU and F30Zn2U) with nonfluorinated analogs (ZnFbU and Zn2U) directly probes the effects of electronic factors on intradimer communication. The major findings of the study are as follows: (1) Energy transfer from the photoexcited Zn porphyrin to the Fb porphyrin is the predominant excited-state reaction in F30ZnFbU, as is also the case for ZnFbU. Energy transfer primarily proceeds via a through-bond process mediated by the diarylethyne linker. Remarkably, the energy-transfer rate is 10 times slower in F30ZnFbU ((240 ps)-1) than in ZnFbU ((24 ps)-1), despite the fact that each has the same diphenylethyne linker. The attenuated energy-transfer rate in the former dimer is attributed to reduced Q-excited-state electronic coupling between the Zn and Fb porphyrins. (2) The rate of hole/electron hopping in the monooxidized bis-Zn complex, [F30Zn2U]+, is .apprx.10-fold slower than that for [Zn2U]+. The slower hole/electron hopping rate in the former dimer reflects strongly attenuated ground-state electronic coupling. The large attenuation in excited- and ground-state electronic communication observed for the F-containing dimers is attributed to a diminution in the electron-exchange matrix elements that stems from stabilization of the a2u porphyrin orbital combined with changes in the electron-d. distribution in this orbital. Stabilization of the porphyrin a2u orbital results in a switch in the HOMO from a2u in ZnFbU to a1u in F30ZnFbU. This orbital reversal diminishes the electron d. at the peripheral positions where the linker is appended. Collectively, the authors' studies clarify the origin of the different energy-transfer rates observed among various multiporphyrin arrays and exemplify the interconnected critical roles of a1u/a2u orbital ordering and linker position in the design of efficient **mol.** photonic **devices.**

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 26, 72, 73, 74

ST energy transfer rate zinc porphyrin; porphyrin copper zinc prepn energy transfer; fluorescence porphyrin zinc complex; electrochem oxidn porphyrin zinc complex

IT Metalloporphyrins
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(copper and zinc; preparation and fluorescence and orbital ordering in relation to electronic communication)

IT Excited singlet state
Excited singlet state
(lifetime of; of porphyrins and their zinc complexes)

IT Resonance Raman spectra
UV and visible spectra
(of porphyrins and their copper and zinc complexes in relation to orbital ordering)

IT Oxidation potential
(of porphyrins and their zinc complexes)

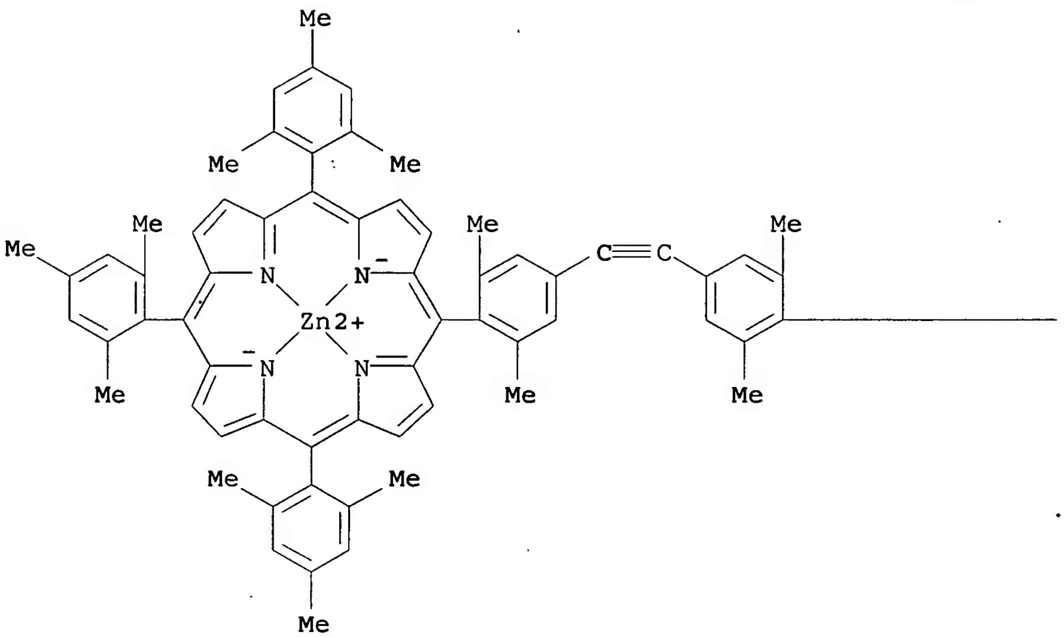
IT Energy transfer
Fluorescence
(of porphyrins and their zinc complexes in relation to orbital ordering)

IT Energy level
(of porphyrins and their zinc porphyrin in relation to electronic communication)

IT ESR (electron spin resonance)
(of zinc porphyrin complexes)

IT Porphyrins
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and fluorescence and orbital ordering in relation to electronic communication)
IT 109-97-7, Pyrrole 653-37-2, Pentafluorobenzaldehyde 15164-44-0, 4-Iodobenzaldehyde 77123-57-0, 4-[2-(Trimethylsilyl)ethynyl]benzaldehyde **199394-17-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of porphyrins and their copper and zinc complexes)
IT **199394-14-4P 199394-15-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and Raman spectra)
IT 199394-10-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and absorption and fluorescence spectra)
IT 199394-16-6P 199394-18-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with copper)
IT 199394-09-7P 199394-11-1P **199394-12-2P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation and coupling reaction with porphyrin and cyclic voltammetry and absorption and fluorescence spectra)
IT 199394-08-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling reaction with zinc porphyrin)
IT **199394-13-3P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation and cyclic voltammetry and fluorescence)
IT **199394-17-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of porphyrins and their copper and zinc complexes)
RN 199394-17-7 HCAPLUS
CN Zinc, [μ-[[5,5'-[1,2-ethynediylbis(2,6-dimethyl-4,1-phenylene)]bis[10,15,20-tris(2,4,6-trimethylphenyl)-21H,23H-porphinato-κN21,κN22,κN23,κN24]](4-)]]di- (9CI) (CA INDEX NAME)

PAGE 1-A



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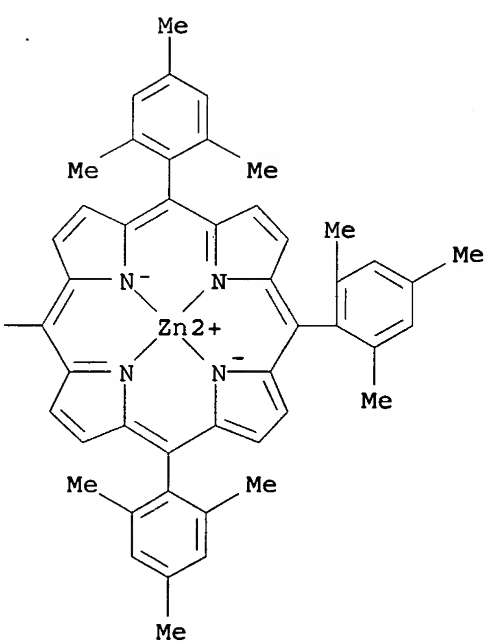


REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 43 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:720588 HCAPLUS
DOCUMENT NUMBER: 128:39885
TITLE: Mesostructure of Evaporated Porphyrin Thin Films: Porphyrin Wheel Formation
AUTHOR(S): Hofkens, Johan; Latterini, Loredana; Vanoppen, Peter; Faes, Herman; Jeuris, Karin; De Feyter, Steven; Kerimo, Josef; Barbara, Paul F.; De Schryver, Frans C.; Rowan, Alan E.; Nolte, Roeland J. M.
CORPORATE SOURCE: Department of Chemistry, Katholieke Universiteit Leuven, Heverlee-Leuven, 3001, Belg.
SOURCE: Journal of Physical Chemistry B (**1997**), 101(49), 10588-10598
CODEN: JPCBFK; ISSN: 1089-5647
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The formation mechanism of ring-shaped assemblies (wheels) obtained from the evaporation of solns. of bis(21H,23H-5(4-pyridyl)-10,15,20-tris(4-hexadecyloxyphenyl)porphyrin)platinum dichloride (PtP) has been studied by a variety of spectroscopic and microscopic techniques, including confocal fluorescence microscopy (CFM), atomic force microscopy (AFM), and near-field scanning optical microscopy (NSOM). Ring-shaped structures have been obtained by deposition of CHCl3 solns. on glass, and a strong dependence of ring shape and size on the initial PtP concentration has been observed
Addition of
methanol (MeOH) to the solution inhibited ring formation if the content of MeOH was higher than 10% in volume Depositions of CHCl3 solns. on graphite instead of on glass exhibited more perfect circular ring structures. Polarization and local time-resolved measurements of the fluorescence at the edge of the rings demonstrated, however, that the rings have similar spectroscopic properties on both **substrates.** Scanning probe microscopy techniques (AFM and NSOM) gave detailed information on the morphol. of the ring. The size of the porphyrin wheels varied from 10 nm to several µm in diameter and between 10 and 200 nm in height. NSOM expts. on the nanoscale optical properties of the samples indicated that the assemblies are organized on the nanometer scale due to small mol. aggregates. Addnl., the effect of the porphyrin (PtP) concentration on the spectroscopic and scattering properties of the PtP solns. revealed that mol. aggregates are formed prior to evaporation The implications of these results on the ring formation mechanism are discussed in this paper.
CC 66-2 (Surface Chemistry and Colloids)
Section cross-reference(s): 26, 28, **36**, **73**, 74
ST porphyrin wheel aggregate thin film; ring assembly methanol chloroform carbon tetrachloride
IT Aggregation
Films
Molecular association
(formation mechanism of ring-shaped assemblies of PtP studied by CFM, AFM, and NSOM)
IT Glass, properties
RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process); USES (Uses)
(formation mechanism of ring-shaped assemblies of PtP studied by CFM, AFM, and NSOM)
IT Porphyrins
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(formation mechanism of ring-shaped assemblies of PtP studied by CFM, AFM, and NSOM)
IT 7782-42-5, Graphite, properties

RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process); USES (Uses)
(formation mechanism of ring-shaped assemblies of PtP studied by CFM, AFM, and NSOM)

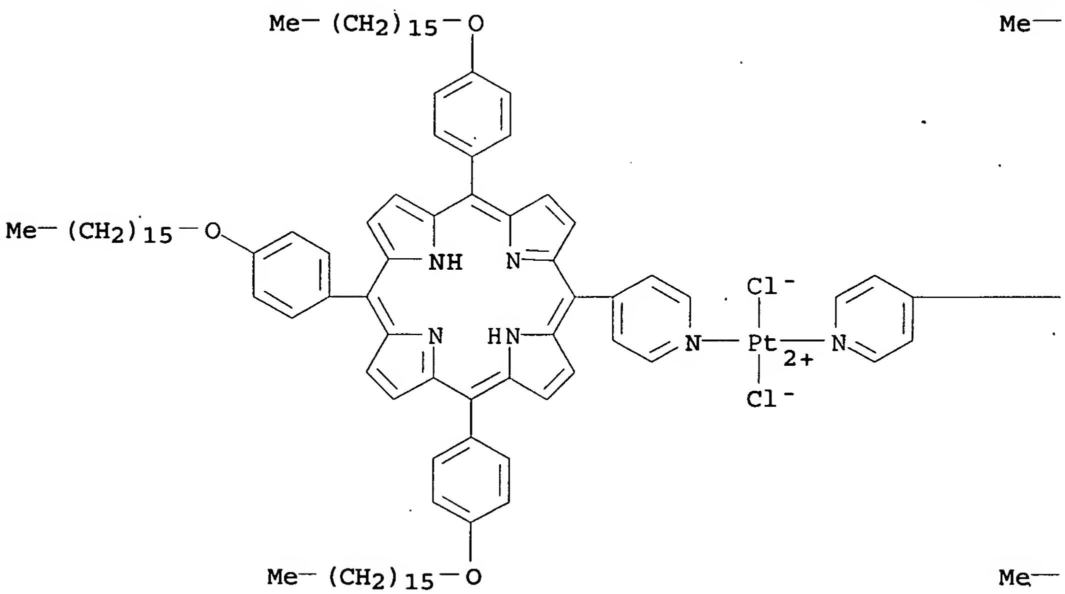
IT 56-23-5, Carbon tetrachloride, properties 67-56-1, Methanol, properties 67-66-3, properties **199739-23-6**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(formation mechanism of ring-shaped assemblies of PtP studied by CFM, AFM, and NSOM)

IT **199739-23-6**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(formation mechanism of ring-shaped assemblies of PtP studied by CFM, AFM, and NSOM)

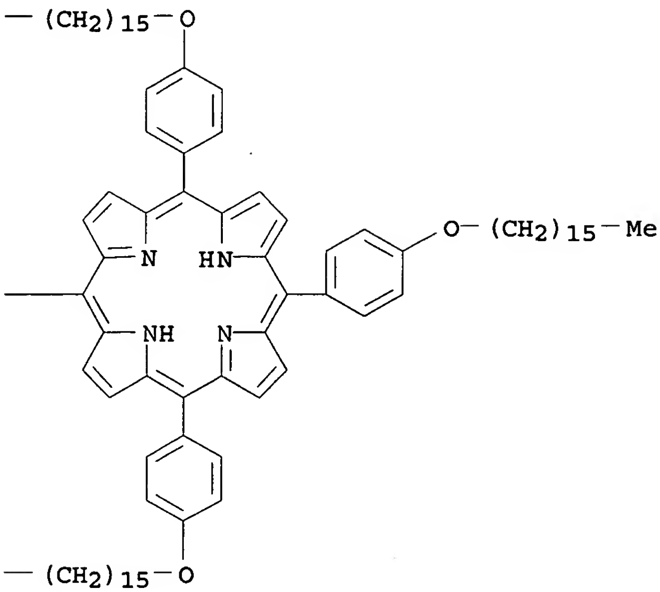
RN 199739-23-6 HCAPLUS

CN Platinum, dichlorobis[5,10,15-tris[4-(hexadecyloxy)phenyl]-20-(4-pyridinyl-κN)-21H,23H-porphine]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 44 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:584592 HCAPLUS
DOCUMENT NUMBER: 127:274610
TITLE: Introduction of Novel Substrate Oxidation into Cytochrome c Peroxidase by Cavity Complementation: Oxidation of 2-Aminothiazole and Covalent Modification of the Enzyme
AUTHOR(S): Musah, Rabi A.; Goodin, David B.
CORPORATE SOURCE: Department of Molecular Biology MB8, Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Biochemistry (**1997**), 36(39), 11665-11674
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The binding and oxidation of an artificial substrate, 2-aminothiazole, by an engineered cavity of cytochrome c peroxidase is described. The W191G mutant has been shown to create a buried cavity into which a number of small heterocyclic compds. will bind [Fitzgerald, M. M., Churchill, M. J., McRee, D. E., & Goodin, D. B. (1994) Biochem. 33, 3807-3818], providing a specific site near the heme from which substrates might be oxidized. In this study, the authors show by titration calorimetry that 2-aminothiazole binds to W191G with a Kd of 0.028 mM at pH 6. A crystal structure at 2.3 Å resolution of W191G in the presence of 2-aminothiazole reveals the occupation of this compound in the cavity, and indicates that it is in van der Waals contact with the heme. The WT enzyme reacts with H2O2 to form Compound ES, in which both the iron center and the Trp-191 side chain are reversibly oxidized. For the W191F (and perhaps the W191G) mutants, the iron is still oxidized, but the second equivalent exists transiently as a radical on the porphyrin before migrating to an alternate protein radical site [Erman, J. E., Vitello, L. B., Mauro, J. M., & Kraut, J. (1989) Biochem. 28, 7992-7995]. Two sep. reactions are observed between

2-aminothiazole and the oxidized centers of W191G. In the one reaction, optical and EPR spectra of the heme are used to show that 2-aminothiazole acts as an electron donor to the ferryl (Fe4+:O) center of W191G to reduce it to the ferric oxidation state. This reaction occurs from within the cavity, as it is not observed for variants that lack this artificial binding site. A second reaction between 2-aminothiazole and peroxide-oxidized W191G, which is much less efficient, results in the specific covalent modification of Tyr-236. Electrospray mass spectra of the W191G after incubation in 2-aminothiazole and H2O2 show a modification of the protein indicative of covalent binding of 2-aminothiazole. The site of modification was determined to be Tyr-236 by CNBr peptide mapping and automated peptide sequencing. The covalent modification is only observed for W191G and W191F which form the alternate radical center. This observation provides an unanticipated assignment of this free radical species to Tyr-236, which is consistent with previous proposals that it is a tyrosine. The oxidation of 2-aminothiazole by W191G represents an example of how the oxidative capacity inherent in the heme prosthetic group and the specific binding behavior of artificial protein cavities can be harnessed and redirected toward the oxidation of organic substrates.

CC 7-5 (Enzymes)

ST substrate oxidn engineered cytochrome c peroxidase; aminothiazole oxidn engineered cytochrome c peroxidase; tyrosine radical cytochrome c peroxidase

IT Enzyme functional sites
(active, artificial; competing oxidation of 2-aminothiazole and covalent modification of active site tyrosine by cytochrome c peroxidase with an engineered substrate-binding cavity)

IT Formation constant
(binding affinity of 2-aminothiazole to cytochrome c peroxidase with an engineered substrate-binding cavity)

IT Oxidation
(biol.; competing oxidation of 2-aminothiazole and covalent modification of active site tyrosine by cytochrome c peroxidase with an engineered substrate-binding cavity)

IT Conformation
Crystal structure
Reaction mechanism
(competing oxidation of 2-aminothiazole and covalent modification of active site tyrosine by cytochrome c peroxidase with an engineered substrate-binding cavity)

IT Radicals, biological studies
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); FMU (Formation, unclassified); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(competing oxidation of 2-aminothiazole and covalent modification of active site tyrosine by cytochrome c peroxidase with an engineered substrate-binding cavity)

IT 9029-53-2, Cytochrome c peroxidase
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(W191G mutant; competing oxidation of 2-aminothiazole and covalent modification of active site tyrosine by cytochrome c peroxidase with an engineered substrate-binding cavity)

IT **14875-96-8**, Heme
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(competing oxidation of 2-aminothiazole and **covalent** modification of active site tyrosine by cytochrome c peroxidase with an engineered **substrate**-binding cavity)

IT 96-50-4, 2-Aminothiazole
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)
(competing oxidation of 2-aminothiazole and covalent modification of active site tyrosine by cytochrome c peroxidase with an engineered substrate-binding cavity)

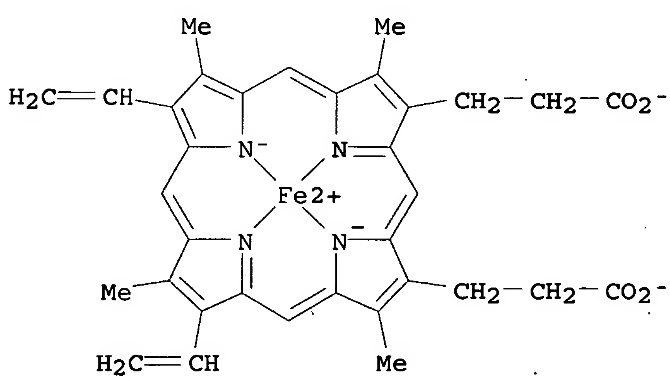
IT 7722-84-1, Hydrogen peroxide, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(competing oxidation of 2-aminothiazole and covalent modification of active site tyrosine by cytochrome c peroxidase with an engineered substrate-binding cavity)

IT 60-18-4, L-Tyrosine, biological studies
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); FMU (Formation, unclassified); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(radical; competing oxidation of 2-aminothiazole and covalent modification of active site tyrosine by cytochrome c peroxidase with an engineered substrate-binding cavity)

IT **14875-96-8**, Heme
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(competing oxidation of 2-aminothiazole and **covalent** modification of active site tyrosine by cytochrome c peroxidase with an engineered **substrate**-binding cavity)

RN 14875-96-8 HCAPLUS

CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-κN21,κN22,κN23,κN24]-, dihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)



●2 H+

L47 ANSWER 45 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:493739 HCAPLUS

DOCUMENT NUMBER: 127:184837

TITLE: Effects of central metal ion (Mg, Zn) and solvent on singlet excited-state energy flow in porphyrin-based nanostructures

AUTHOR(S): Li, Feirong; Gentemann, Steve; Kalsbeck, William A.;

Seth, Jyoti; Lindsey, Jonathan S.; Holten, Dewey; Bocian, David F.
CORPORATE SOURCE: Department of Chemistry, North Carolina State University, Raleigh, NC, 27695-8204, USA
SOURCE: Journal of Materials Chemistry (**1997**), 7(7), 1245-1262
CODEN: JMACEP; ISSN: 0959-9428
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Zinc porphyrins were widely used as surrogates for chlorophyll (which contains magnesium) in photosynthetic model systems and **mol.** photonic **devices.** To compare the photodynamic behavior of Mg- and Zn-porphyrins, dimeric and star-shaped pentameric arrays comprised of free-base (Fb) and Mg- or Zn-porphyrins with intervening diarylethyne linkers were prepared A modular building block approach was used to couple ethynyl- or iodo-substituted porphyrins in defined metalation states (Fb, Mg or Zn) via a Pd-catalyzed reaction in 2-6 h. The resulting arrays are purified in 45-80% overall yields by combinations of size exclusion chromatog. and adsorption chromatog. (≥95% purity). High solubility of the arrays in organic solvents facilitates chemical and spectroscopic characterization. The star-shaped Mg4Fb- and Zn4Fb-pentamers, where the Fb-porphyrin is at the core of the array, have pairwise interactions similar to those of dimeric MgFb- and ZnFb-arrays. The arrays were studied by static and time-resolved absorption and fluorescence spectroscopy, as well as resonance Raman spectroscopy. The major findings include the following. (1) The rate of singlet excited-state energy transfer from the Mg-porphyrin to the Fb-porphyrin [(31 ps)-1] is comparable to that from the Zn-porphyrin to the Fb-porphyrin [(26 ps)-1] in the dimeric arrays. Qual. similar results were obtained for the star-shaped pentamers. The similar rates of energy transfer for the Mg- and Zn-containing arrays are attributed to the fact that the electronic coupling between the metalloporphyrin and Fb-porphyrin is approx. the same for Mg- vs. Zn-containing arrays. (2) The quantum yield of energy transfer is slightly higher in the Mg- arrays (99.7%) than in the Zn-arrays (99.0%) due to the longer inherent lifetime of Mg-porphyrins (10 ns) compared with Zn-porphyrins (2.5 ns). (3) The rate of energy transfer and the magnitude of the electronic coupling are essentially independent of the solvent polarity and the coordination geometry of the metalloporphyrin (four- or five-coordinate for Zn-porphyrins, five- or six-coordinate for Mg-porphyrins). (4) Polar solvents diminish the fluorescence yield and lifetime of the excited Fb-porphyrin in arrays containing either Mg- or Zn-porphyrins. These effects are attributed to charge-transfer quenching of the Fb-porphyrin by the adjacent metalloporphyrin rather than to changes in electronic coupling. The magnitude of the diminution is greater for the Mg-containing arrays, which is due to the greater driving force for charge separation (5) The Zn-containing arrays are quite robust while the Mg-containing arrays are slightly labile toward demetalation and photooxidn. Taken together, these results indicate that porphyrin-based nanostructures having high energy-transfer efficiencies can be constructed from either Mg- or Zn-porphyrins. However, Mg-containing arrays may be superior in situations where a succession of energy-transfer steps occurs (due to a slightly higher yield per step) or where charge transfer is a desirable feature. However, Zn-porphyrins are better suited when it is desirable to avoid charge transfer quenching reactions. Accordingly, the merits of constructing a device from Mg- vs. Zn-containing porphyrins will be determined by the interplay of all of the above factors.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 11, 73, 74

ST porphyrin magnesium zinc prepn energy flow; magnesium diarylethyne linked porphyrinato prepn photochem; zinc diarylethyne linked porphyrinato prepn photochem; energy flow magnesium zinc porphyrinato array; photochem magnesium zinc diarylethyne linked porphyrinato; Raman magnesium zinc diarylethyne linked porphyrinato; fluorescence magnesium zinc diarylethyne linked porphyrinato; charge transfer kinetics diarylethyne linked metalloporphyrinato; chlorophyll model diarylethyne linked metalloporphyrin photochem; nanostructure magnesium zinc diarylethyne linked porphyrinato

IT Nanostructures
(effects of central metal ion (Mg, Zn) and solvent on singlet excited-state energy flow in porphyrin-based nanostructures)

IT Chlorophylls, preparation
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(effects of central metal ion (Mg, Zn) and solvent on singlet excited-state energy flow in porphyrin-based nanostructures as models for)

IT Electron transfer kinetics
Fluorescence decay
Singlet state transition
(of magnesium and zinc diarylethyne-linked porphyrinate dimeric and star-shaped pentameric array complexes)

IT Fluorescence
Resonance Raman spectra
UV and visible spectra
(of magnesium and zinc monomeric and diarylethyne-linked porphyrinate dimeric and star-shaped pentameric array complexes)

IT Solvent effect
(on photodynamics of energy transfer and fluorescence of magnesium and zinc diarylethyne-linked porphyrinate dimeric and star-shaped pentameric array complexes)

IT Intramolecular energy transfer
(photochem.; of magnesium and zinc diarylethyne-linked porphyrinate dimeric and star-shaped pentameric array complexes)

IT Fluorescence quenching
(polar solvent effect on fluorescence quenching of magnesium and zinc diarylethyne-linked porphyrinate dimeric and star-shaped pentameric array complexes)

IT Metalloporphyrins
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation, UV-visible, Raman and fluorescence spectra, and energy-transfer rate consts. and yields of magnesium and zinc diarylethyne-linked porphyrinate dimeric and star-shaped pentameric array complexes)

IT Photosystems
(reaction center; of magnesium and zinc diarylethyne-linked porphyrinate dimeric and star-shaped pentameric array complexes)

IT Photoinduced energy transfer
(singlet excited-state, of magnesium and zinc diarylethyne-linked porphyrinate dimeric and star-shaped pentameric array complexes)

IT 917-23-7, 5,10,15,20-Tetraphenylporphyrin 14074-80-7, (5,10,15,20-Tetraphenylporphyrinato)zinc 14640-21-2, (5,10,15,20-Tetraphenylporphyrinato)magnesium 145362-97-6, 5,10,15,20-Tetrakis{4-[2-(trimethylsilyl)ethynyl]phenyl}porphyrin
RL: PRP (Properties)
(UV-visible and fluorescence spectra)

IT 160682-08-6, 5,10,15-Trimesityl-20-{4-[2-(trimethylsilyl)ethynyl]phenyl}po rphyrin

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(UV-visible and fluorescence spectra and reaction with magnesium iodide)

IT 184153-94-4, (5,10,15-Trimesityl-20-{4-[2-(trimethylsilyl)ethynyl]phenyl}porphyrinato)zinc
RL: PRP (Properties)
(UV-visible, Raman and fluorescence spectra)

IT **160700-59-4**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(UV-visible, Raman and fluorescence spectra, and energy-transfer rate constant and yield)

IT 603-32-7, Triphenylarsine 51364-51-3, Tris(dibenzylideneacetone)dipalladium
RL: CAT (Catalyst use); USES (Uses)
(for preparation of magnesium and zinc diarylethyne-linked porphyrinate dimeric and star-shaped pentameric array complexes)

IT 29162-74-1, 5,10,15,20-Tetrakis(4-iodophenyl)porphyrin
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of magnesium and zinc tetrakis(trimesitylporphinylphenylethynylphenyl)porphyrinato tetranuclear complexes)

IT 160682-10-0, 5-(4-Iodophenyl)-10,15,20-trimesitylporphyrin
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of magnesium bis(trimesitylporphinyl)diphenylacetylene complex)

IT 194035-41-1P, 4-(5,10,15-Trimesityl-20-porphinyl)-4'-(5,10,15-trimesityl-20-porphinyl)-diphenylacetylene
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of magnesium bis(trimesitylporphinyl)diphenylacetylene dinuclear complex)

IT 194035-39-7P, (5,10,15-Trimesityl-20-(4-ethynylphenyl)porphyrinato)magnesium
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of magnesium tetrakis(trimesitylporphinylphenylethynylphenyl)porphyrinato tetranuclear complex)

IT 150152-74-2, (5,10,15-Trimesityl-20-(4-ethynylphenyl)porphyrinato)zinc
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of zinc tetrakis(trimesitylporphinylphenylethynylphenyl)porphyrinato tetranuclear complex)

IT 194035-53-5 194035-57-9 194035-58-0 194035-61-5 194035-63-7 194035-64-8 194035-65-9 **194035-66-0** **194035-70-6**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(formation and UV-visible and fluorescence spectra)

IT 61477-51-8 61477-52-9 61483-54-3 61483-89-4 67820-00-2 194035-43-3 194035-44-4 194035-45-5 194035-47-7 194035-49-9 194035-54-6 194035-59-1 194035-62-6
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(formation and UV-visible spectrum)

IT **194035-67-1** **194035-68-2** **194035-69-3** **194035-71-7** **194035-72-8** **194035-73-9** **194035-74-0**
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)
(formation, UV-visible and fluorescence spectra, and energy-transfer rate constant and yield)

IT 194100-81-7P 194100-82-8P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and UV-visible and fluorescence spectra, and energy-transfer rate constant and yield)

IT **194035-40-0P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and UV-visible, Raman and fluorescence spectra, and energy-transfer rate constant and yield)

IT **194035-42-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

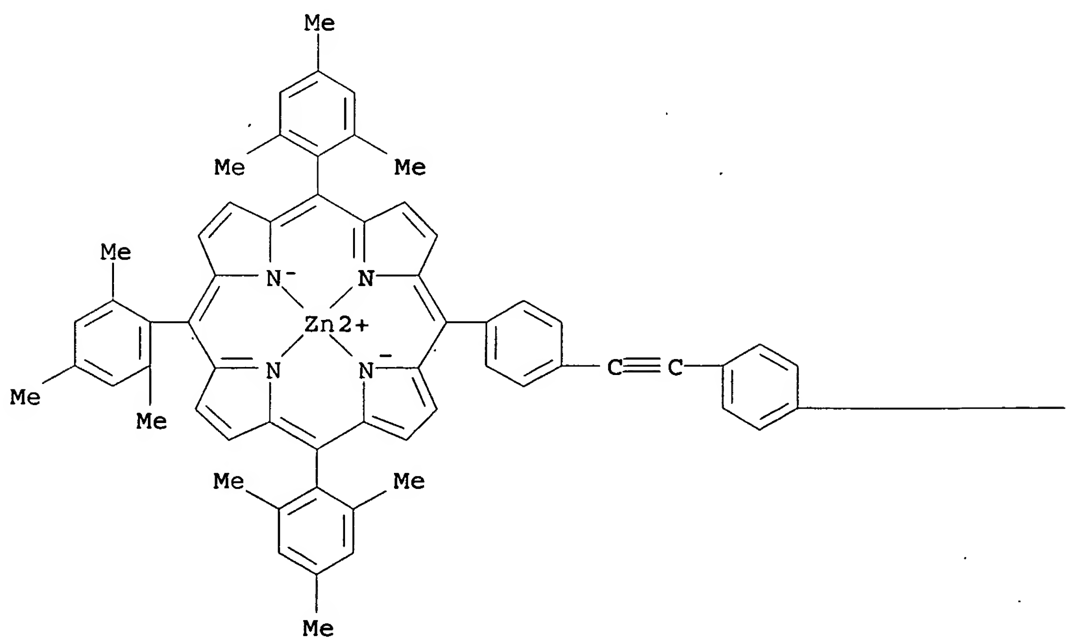
IT 194035-38-6P, (5,10,15-Trimesityl-20-{4-[2-(trimethylsilyl)ethynyl]phenyl}porphyrinato)magnesium
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, UV-visible, Raman and fluorescence spectra, and reaction with tetrabutylammonium fluoride)

IT **160700-59-4**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(UV-visible, Raman and fluorescence spectra, and energy-transfer rate constant and yield)

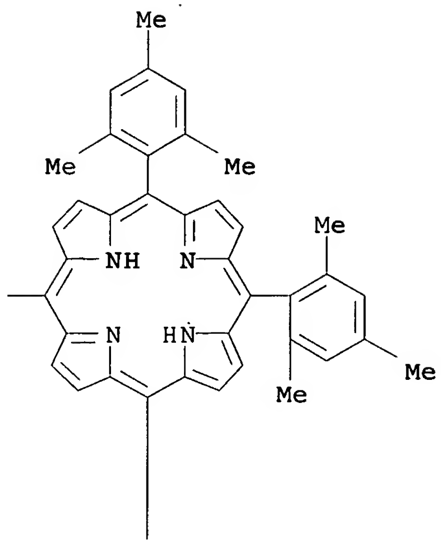
RN 160700-59-4 HCAPLUS

CN Zinc, [10,15,20-tris(2,4,6-trimethylphenyl)-5-[4-[[4-[10,15,20-tris(2,4,6-trimethylphenyl)-21H,23H-porphin-5-yl]phenyl]ethynyl]phenyl]-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-2)-
(9CI) (CA INDEX NAME)

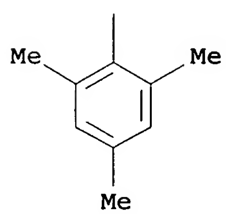
PAGE 1-A



PAGE 1-B



PAGE 2-B



REFERENCE COUNT: 103 THERE ARE 103 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 46 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:657117 HCAPLUS
DOCUMENT NUMBER: 126:18688
TITLE: Soluble Synthetic Multiporphyrin Arrays. 1. Modular Design and Synthesis
AUTHOR(S): Wagner, Richard W.; Johnson, Thomas E.; Lindsey, Jonathan S.
CORPORATE SOURCE: Department of Chemistry, North Carolina State University, Raleigh, NC, 27695-8204, USA
SOURCE: Journal of the American Chemical Society (**1996**), 118(45), 11166-11180
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:18688

AB A set of porphyrin building blocks has been developed for the construction of light-harvesting model compds. and related **mol.** photonic **devices.** The porphyrins are facially encumbered to enhance solubility in organic solvents, are employed in a defined metalation state (free base (Fb) or zinc chelate), and bear peripheral functional groups such as iodo or ethyne for joining the porphyrins via covalent bonds. The coupling of an iodophenylporphyrin and an ethynylphenylporphyrin via mild Pd-mediated reactions (2-4 mM of each porphyrin in toluene/triethylamine (5:1) with Pd2(dba)3 and AsPh3 at 35 °C for 2 h) yields the corresponding diphenylethyne-linked multiporphyrin array in 70-80% yield. The arrays are easily purified by a sequence of flash silica chromatog., preparative size exclusion chromatog., and gravity elution silica chromatog. The diphenylethyne linkers give a center-to-center separation of the porphyrins of .apprx.20 Å. Model light-harvesting compds. are easily prepared using Zn and Fb porphyrin building blocks. In order to investigate the role of the linker in through-bond electronic communication, and the effect of through-bond electronic communication on the rates and yields of photoinduced energy transfer in the arrays, four ZnFb dimers have been prepared that have a systematic increase in steric hindrance in the diphenylethyne unit. The presence of steric hindrance inhibits rotation of the Ph group toward coplanarity with the porphyrin, thereby modulating the electronic communication. A linear ZnFbZn trimer and a right-angle ZnFbZn trimer have been prepared to probe the effects of geometry on electronic communication pathways. A linear ZnZnFb trimer has been synthesized to investigate the photodynamics of energy migration among isoenergetic zinc porphyrins. These multiporphyrin arrays have sufficient solubility (.apprx.5 mM) for routine handling in organic solvents such as toluene,
CH2Cl2, or CHCl3, and can be examined spectroscopically (1-10 μM) in diverse solvents such as THF, acetone, DMSO, and castor oil. This building block approach should make diverse multiporphyrin arrays readily available.

CC 26-7 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 22

ST porphyrin light harvesting model compd prepn; **mol** photonic **device** porphyrin contg prepn; palladium mediated coupling iodophenylporphyrin ethynylphenylporphyrin; diphenylethyne linked multiporphyrin array prepn property; electronic communication through bond multiporphyrin array; photoinduced energy transfer multiporphyrin array; rotation inhibition steric hindrance multiporphyrin array; photodynamics migration energy multiporphyrin array; soly multiporphyrin array

IT Photosystems
(light-harvesting complex; preparation of multiporphyrin arrays as light-harvesting model compds. and related **mol.** photonic **devices**)

IT Solubility
(preparation of facially-encumbered multiporphyrin arrays as highly soluble light-harvesting model compds.)

IT Steric hindrance
(preparation of multiporphyrin arrays as light-harvesting model compds. and related **mol.** photonic **devices**)

IT Photosystems
(reaction center, synthetic; preparation of multiporphyrin arrays as light-harvesting model compds. and related **mol.** photonic **devices**)

IT Metalloporphyrins
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(zinc; preparation of multiporphyrin arrays as light-harvesting model compds. and related **mol.** photonic **devices**)

IT **160700-60-7**

RL: PRP (Properties)
(preparation of multiporphyrin arrays as light-harvesting model compds. and related **mol.** photonic **devices**)

IT 184153-94-4P 184153-97-7P 184153-99-9P **184154-14-1P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of multiporphyrin arrays as light-harvesting model compds. and related **mol.** photonic **devices**)

IT 160682-08-6P **160700-59-4P 183281-29-0P**
184154-13-0P 184154-15-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of multiporphyrin arrays as light-harvesting model compds. and related **mol.** photonic **devices**)

IT 109-97-7, Pyrrole 557-34-6, Zinc acetate 591-50-4, Iodobenzene 3392-97-0, 2,6-Dimethoxybenzaldehyde 4102-53-8, 2,6-Dimethyl-4-iodoaniline 15164-44-0, 4-Iodobenzaldehyde 29162-74-1, 5,10,15,20-Tetrakis(4-iodophenyl)porphyrin 77123-57-0, 4-[2-(Trimethylsilyl)ethynyl]benzaldehyde 150174-04-2 159152-14-4
166186-42-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of multiporphyrin arrays as light-harvesting model compds. and related **mol.** photonic **devices**)

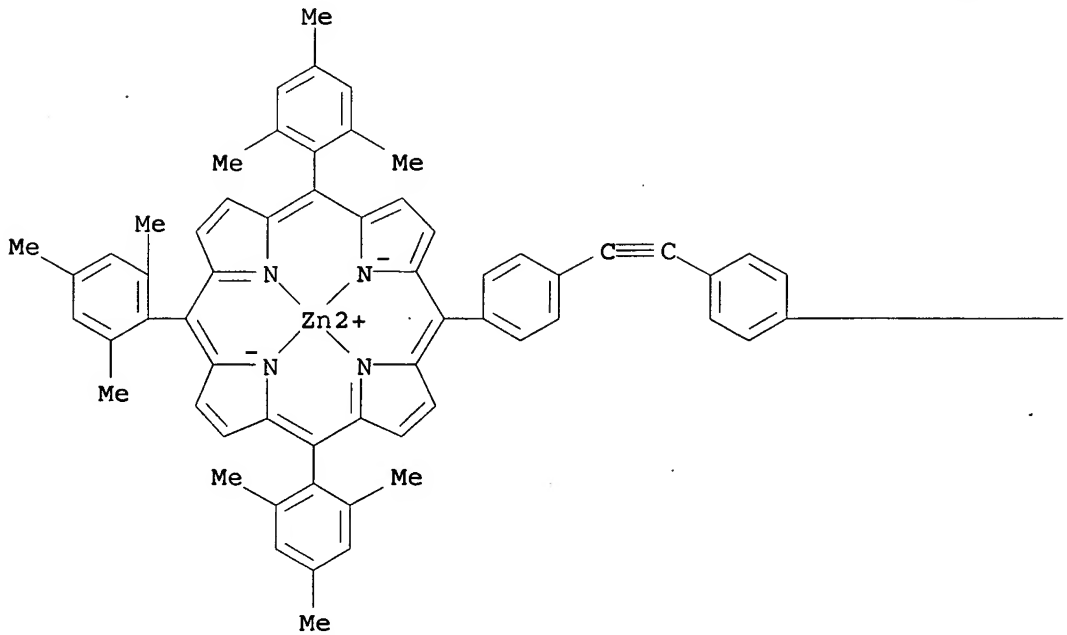
IT 487-68-3P, Mesitaldehyde 536-74-3P, Phenylacetylene 1066-54-2P, Trimethylsilylacetylene 5769-33-5P, 4-Bromo-2,6-dimethylbenzaldehyde 150152-74-2P 159152-22-4P 160682-00-8P, 4-Iodo-2,6-dimethylbenzonitrile 160682-01-9P, 4-Iodo-2,6-dimethylbenzaldehyde 160682-10-0P 184153-93-3P 184154-01-6P 184154-03-8P 184154-06-1P 184154-08-3P 184154-09-4P 184154-11-8P 184154-12-9P
184154-20-9P 184154-22-1P 184154-23-2P
184154-24-3P 184154-25-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of multiporphyrin arrays as light-harvesting model compds. and related **mol.** photonic **devices**)

IT 159152-21-3P 159501-21-0P 159501-24-3P 159606-06-1P
183281-30-3P 184153-95-5P **184154-17-4P**
184154-18-5P 184154-19-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of multiporphyrin arrays as light-harvesting model compds. and related **mol.** photonic **devices**)

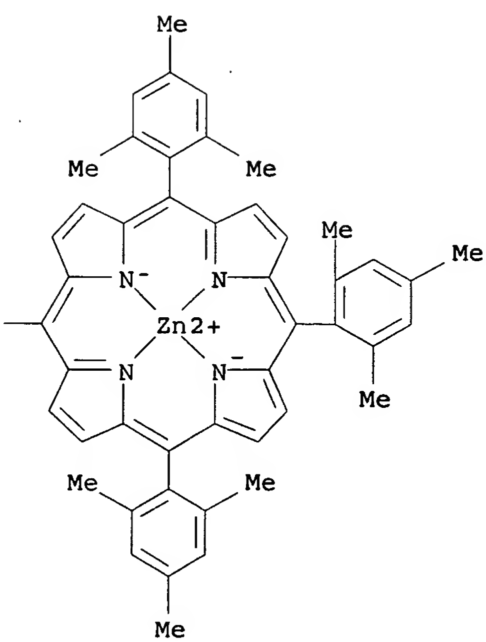
IT **160700-60-7**
RL: PRP (Properties)
(preparation of multiporphyrin arrays as light-harvesting model compds. and related **mol.** photonic **devices**)

RN 160700-60-7 HCAPLUS
CN Zinc, [μ-[[5,5'-(1,2-ethynediyldi-4,1-phenylene)bis[10,15,20-tris(2,4,6-trimethylphenyl)-21H,23H-porphinato-κN21,κN22,κN23,.kapp a.N24]](4-)]]di- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 106 THERE ARE 106 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 47 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:539053 HCAPLUS
DOCUMENT NUMBER: 125:260693
TITLE: Optical studies of dye-coated superconductor junctions
AUTHOR(S): Savoy, Steven; Eames, Sara; Jurbergs, David; Zhao, Jianai; McDevitt, John T.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Texas, Austin, TX, 78712, USA
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (**1996**), 2696(Pt. B, Spectroscopic Studies of Superconductors, Pt. B), 672-679
CODEN: PSISDG; ISSN: 0277-786X
PUBLISHER: SPIE-The International Society for Optical Engineering
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The preparation and characterization of a new generation of optical sensors fabricated from high-temperature superconductor (HTSC) thin films is reported herein. These new hybrid **devices** are fashioned using HTSC thin films which are coated with organic dye overlayers. These systems respond selectively to those wavelengths which are absorbed strongly by the mol. dye. Methods for fabricating the superconductor element and depositing the dye layer are discussed. Also, resistivity vs. temperature measurements before and after dye deposition were used to characterize these hybrid structures. The unique optical response properties of these hybrid sensors are also detailed.

CC 73-11 (**Optical**, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 76

ST dye coated superconductor junction optical sensor; barium copper yttrium oxide superconductor junction

IT Dyes
Superconductors
(optical studies and applications of dye-coated Ba2Cu3YO7-x superconductor junctions)

IT Superconductor **devices**
(junctions, optical studies and applications of dye-coated Ba2Cu3YO7-x superconductor junctions)

IT Sensors
(optical, optical studies and applications of dye-coated Ba2Cu3YO7-x superconductor junctions)

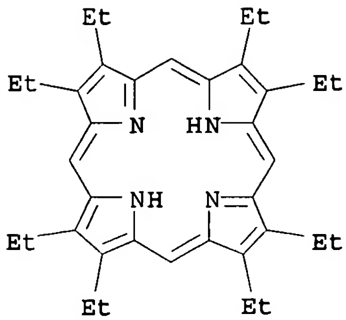
IT 1309-48-4, Magnesium oxide, uses
RL: **DEV (Device component use)**; USES (Uses)
(optical studies of dye-coated Ba2Cu3YO7-x superconductor junctions on MgO substrate)

IT 574-93-6, Phthalocyanine 989-38-8, Rhodamine 6G **2683-82-1**, Octaethylporphyrin 109064-29-1D, Barium copper yttrium oxide ba2cu3yo7, oxygen-deficient
RL: **DEV (Device component use)**; PRP (Properties); USES (Uses)
(optical studies of dye-coated Ba2Cu3YO7-x superconductor junctions on MgO **substrate**)

IT **2683-82-1**, Octaethylporphyrin
RL: **DEV (Device component use)**; PRP (Properties); USES (Uses)
(optical studies of dye-coated Ba2Cu3YO7-x superconductor junctions on MgO **substrate**)

RN 2683-82-1 HCAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octaethyl- (9CI) (CA INDEX NAME)



L47 ANSWER 48 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:246712 HCAPLUS
DOCUMENT NUMBER: 122:20978
TITLE: Articles including thin-film monolayers and multilayers
INVENTOR(S): Li, Dequan; Swanson, Basil I.
PATENT ASSIGNEE(S): United States Dept. of Energy, USA
SOURCE: U. S. Pat. Appl., 19 pp. Avail. NTIS Order No. PAT-APPL-7-874,890.
CODEN: XAXXAV
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 874890	A0	19941015	US 1992-874890	19920428 <--
US 5397642	A	19950314		

PRIORITY APPLN. INFO.: US 1992-874890 19920428 <--

AB The articles include: (a) a base substrate having an oxide surface layer, and a multidentate ligand, capable of binding a metal ion, attached to the oxide surface layer of the base substrate; (b) a base substrate having an oxide surface layer, a multidentate ligand, capable of binding a metal atom, attached to the oxide surface layer of the base substrate, and a metal species attached to the multidentate ligand; (c) a base substrate having an oxide surface layer, a multidentate ligand, capable of binding a metal ion, attached to the oxide surface layer of the base substrate, a metal species attached to the multidentate ligand, and a multifunctional organic ligand attached to the metal species; and (d) a base substrate having an oxide surface layer, a multidentate ligand, capable of binding a metal ion, attached to the oxide surface layer of the base substrate, a metal species attached to the multidentate ligand, a multifunctional organic ligand attached to the metal species, and a second metal species attached to the multifunctional organic ligand. Such articles are useful in detecting the presence of a selected target species, as nonlinear optical materials, or as scavengers for selected target species.

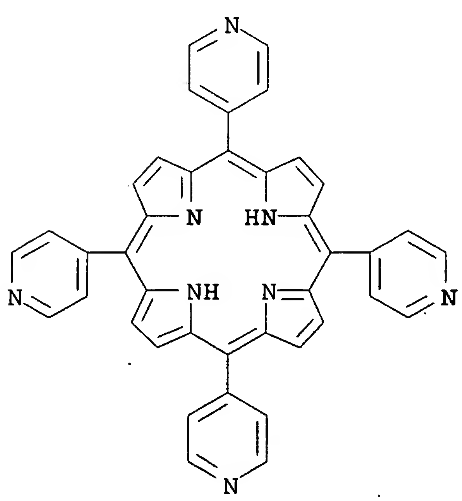
CC 75-1 (Crystallography and Liquid Crystals)
Section cross-reference(s): **73**, 78, 79, 80

ST thin film sensor optical material scavenger

IT Scavengers
Sensors
(articles including thin-film monolayers and multilayers as)

IT Optical materials
(articles including thin-film monolayers and multilayers as nonlinear)

IT 13688-90-9 **16834-13-2**, 5,10,15,20-Tetra(4-pyridyl)-21H,23H-porphine
RL: **DEV (Device component use)**; PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(for coating quartz **substrate** in articles including thin-film monolayers and multilayers)
IT 84127-79-7, N-[3-Trimethoxysilyl)propyl]ethylenediaminetriacetate
RL: **DEV (Device component use)**; RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(for coating quartz substrate in articles including thin-film monolayers and multilayers)
IT 159666-36-1DP, silica-bound
RL: **DEV (Device component use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(for coating quartz substrate in articles including thin-film monolayers and multilayers)
IT 159666-37-2D, silica-bound
RL: RCT (Reactant); RACT (Reactant or reagent)
(for coating quartz substrate in articles including thin-film monolayers and multilayers)
IT 15694-44-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of)
IT 159644-57-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 14808-60-7, Quartz, uses
RL: **DEV (Device component use)**; USES (Uses)
(substrate in articles including thin-film monolayers and multilayers)
IT **16834-13-2**, 5,10,15,20-Tetra(4-pyridyl)-21H,23H-porphine
RL: **DEV (Device component use)**; PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(for coating quartz **substrate** in articles including thin-film monolayers and multilayers)
RN 16834-13-2 HCAPLUS
CN 21H,23H-Porphine, 5,10,15,20-tetra-4-pyridinyl- (9CI) (CA INDEX NAME)



L47 ANSWER 49 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:44946 HCAPLUS
DOCUMENT NUMBER: 122:105489
TITLE: Porphyrin building blocks for modular construction of bioorganic model systems
AUTHOR(S): Lindsey, Jonathan S.; Prathapan, Sreedharan; Johnson, Thomas E.; Wagner, Richard W.
CORPORATE SOURCE: Dep. Chem., Carnegie Mellon Univ., Pittsburgh, PA, 15213, USA
SOURCE: Tetrahedron (**1994**), 50(30), 8941-68
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors outline a modular building block strategy for the covalent assembly of porphyrin-containing model systems. Mol. design issues for the synthesis of porphyrin dimers, dye-porphyrin dyads, and multi-porphyrin arrays have been used to guide the development of this approach. The major design constraints are to achieve directed coupling of free base and/or metalloporphyrin building blocks in dilute solution under non-acidic non-metalating conditions. A set of 24 porphyrin building blocks has been synthesized. The porphyrins are prepared by reaction of substituted benzaldehydes with pyrrole using the two-step one-flask room temperature porphyrin synthesis. Routes to 7 substituted aldehydes are described. Each porphyrin bears one or four functional groups, and many also are facially-encumbered in order to achieve increased solubility Twelve functional groups that meet the design criteria include those that can be reacted directly in coupling reactions such as active esters, α-chloroacetamido, benzoyl, and iodo groups, and others that require deprotection prior to coupling, such as phthalimidomethyl, FMOC-prolyl, trimethylsilylethynyl, dithiolane, methoxycarbonyl, and trimethylsilylethoxycarbonyl groups. The synthesis of 13 porphyrin dimers and dye-porphyrin dyads has been explored as a testbed for refining strategies for the synthesis of **mol. devices** containing multiple porphyrins and other components. The coupling strategies investigated have yielded dimers or dyads with subunits linked by amide, butadiyne, ethyne, or thiourea groups. This building block approach should enable rapid assembly of architecturally-defined porphyrin-based model systems.
CC 26-7 (Biomolecules and Their Synthetic Analogs)
ST porphyrin building block bioorg system
IT 71989-31-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of (aminophenyl)dithiolane)
IT 160682-19-9 160682-20-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with amino porphyrin)
IT 771-61-9, Pentafluorophenol 2916-68-9, 2-(Trimethylsilyl)ethanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with formylbenzoic acid)
IT 619-66-9, 4-Formylbenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with pentafluorophenol)
IT 5769-33-5, 4-Bromo-2,6-Dimethylbenzaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with (trimethylsilyl)acetylene)
IT 1066-54-2, (Trimethylsilyl)acetylene
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with bromobenzaldehyde)
IT 150174-04-2 150174-05-3 160700-62-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with porphyrin)

IT 150152-74-2 160700-61-8 160734-19-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with porphyrins)
IT 67605-64-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with zinc-porphyrin)
IT 104-53-0, Hydrocinnamaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with benzaldehyde and pyrrole)
IT 555-16-8, 4-Nitrobenzaldehyde, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with ethanedithiol)
IT 122-78-1, Phenylacetaldehyde 1074-12-0, Phenylglyoxal 15164-44-0, 4-Iodobenzaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with pyrrole)
IT 830-79-5, 2,4,6-Trimethoxybenzaldehyde 3392-97-0, 2,6-Dimethoxybenzaldehyde 77123-57-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with pyrrole and benzaldehyde derivative)
IT 66-25-1, Hexanal
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with pyrrole and dithiolane derivative)
IT 78784-21-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with pyrrole and hexanal)
IT 100-52-7, Benzaldehyde, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with pyrrole and hydrocinnamaldehyde)
IT 1571-08-0, Methyl 4-formylbenzoate 51359-79-6 60444-78-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with pyrrole and mesitaldehyde)
IT 104-87-0, p-Tolualdehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with pyrrole and phenylglyoxal)
IT 109-97-7, Pyrrole
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reactions of)
IT 487-68-3, Mesitaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reactions of, with pyrrole and benzaldehydes)
IT 4102-53-8, 2,6-Dimethyl-4-iodoaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(diazotization and reduction of)
IT 94838-73-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of)
IT 145363-20-8P 150021-14-0P 160682-06-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with porphyrin)
IT 145363-21-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with zinc-porphyrin)
IT 88679-81-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyanation of)

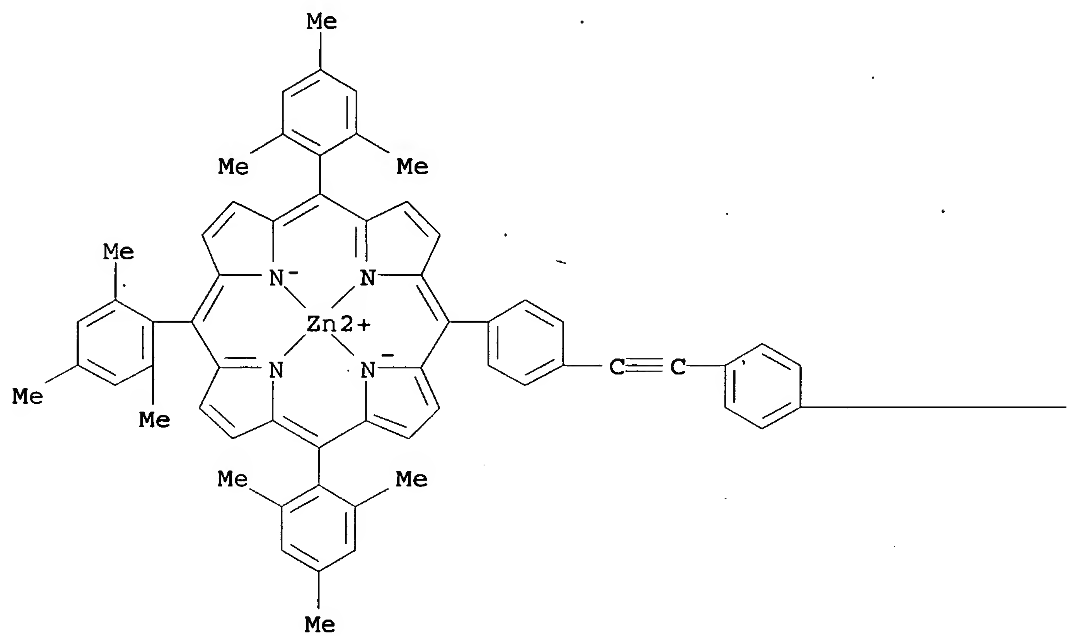
IT 160682-01-9P 160682-03-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with pyrrole)
IT 160681-99-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with pyrrole and benzaldehydes)
IT 160681-98-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with pyrrole and dimethyoxybenzaldehyde)
IT 159152-22-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with pyrrole and iodobenzaldehyde)
IT 160681-97-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with pyrrole and mesitaldehyde)
IT 145363-15-1P 160681-96-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
IT 150021-13-9P 160682-08-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desilylation of)
IT 145363-16-2P 145363-17-3P 157870-16-1P 160682-02-0P 160682-14-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT **160700-59-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and metalation of)
IT 41159-02-8P 160682-00-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 29162-74-1P 36729-83-6P 97562-32-8P 145362-97-6P 145362-98-7P
145363-12-8P 145363-13-9P 145363-14-0P 145363-18-4P 145363-25-3P
146023-48-5P 150021-16-2P **159501-22-1P** 159501-25-4P
160682-04-2P 160682-05-3P 160682-07-5P 160682-09-7P 160682-10-0P
160682-11-1P 160682-12-2P 160682-13-3P 160682-15-5P 160682-16-6P
160682-17-7P 160682-18-8P **160700-55-0P** **160700-56-1P**
160700-57-2P **160700-58-3P** **160700-60-7P**
160734-18-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 160681-95-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, deprotection, and cyclocondensation of, with pyrrole and mesitaldehyde)
IT **145994-86-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, zinc insertion, and demetalation of)
IT **160700-59-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and metalation of)

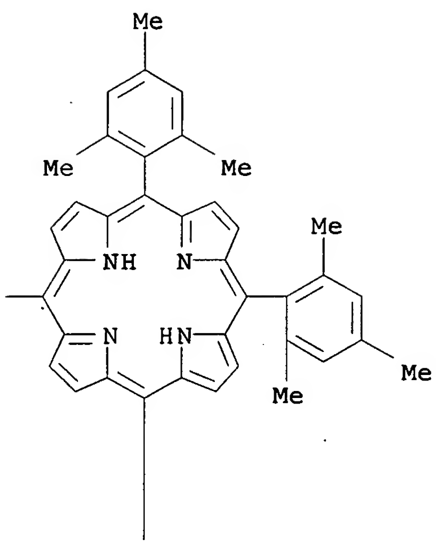
RN 160700-59-4 HCAPLUS

CN Zinc, [10,15,20-tris(2,4,6-trimethylphenyl)-5-[4-[[4-[10,15,20-tris(2,4,6-trimethylphenyl)-21H,23H-porphin-5-yl]phenyl]ethynyl]phenyl]-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-2)-
(9CI) (CA INDEX NAME)

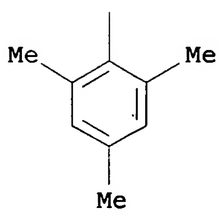
PAGE 1-A



PAGE 1-B



PAGE 2-B



L47 ANSWER 50 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:22384 HCAPLUS
DOCUMENT NUMBER: 120:22384
TITLE: Synthesis and film-forming properties of metal complexes of octadecyl ethers of 5,10,15,20-tetrakis(4-hydroxyphenyl)porphyrin
AUTHOR(S): Bonnett, Raymond; Ioannou, Stella; James, Andrew G.; Pitt, Christopher W.; Soe, Moe M. Z.
CORPORATE SOURCE: Dep. Chem., Queen Mary and Westfield Coll., London, E1 4NS, UK
SOURCE: Journal of Materials Chemistry (1993), 3(8), 793-9
CODEN: JMACEP; ISSN: 0959-9428
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Metal complexes [AlIII, FeIII, CoII, NiII, CuII, ZnII, CdII, and PtII] of various octadecyl ethers of 5,10,15,20-tetrakis(4-hydroxyphenyl)porphyrin were prepared and characterized. The metalloporphyrins are examined for their ability to form layers using the Langmuir technique, and pressure-area

isotherms are presented. Multilayers on glass **substrates** are made in suitable cases using the Langmuir-Blodgett method. Complexes of the tris(octadecyl) ether generally give films with favorable properties although the Al(III) complex, which is dimeric, does not. In certain cases where the pure metalloporphyrin gives unsatisfactory results, the film can be improved using a stabilizer such as stearic acid. The absorption maximum of the films are determined before and after exposure to sensor
gases (Cl2, HCl, NO2) and after further exposure to hydrazine vapor ('hydrazine reset'), and compared with solution spectra.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 59, 66, **73**, 79

ST film transition metal octadecyl ether hydroxyphenylporphyrin; transition metal octadecyl ether hydroxyphenylporphyrin complex; gas sensor metal octadecyl ether hydroxyphenylporphyrin; porphyrin hydroxyphenyl octadecyl ether metal complex; Langmuir Blodgett film metal porphyrin complex

IT Coating process
(of metal complexes with octadecyl ether derivs. of (hydroxyphenyl)porphyrins)

IT Films
(of metal complexes with octadecyl ether derivs. of (hydroxyphenyl)porphyrins, optical properties and potential use of, in gas sensors)

IT Transition metals, compounds
RL: SPN (Synthetic preparation); PREP (Preparation)
(aryl porphyrin complexes, octadecyl ether derivs., preparation and film formation and potential use of, in gas sensors)

IT Porphyrins
RL: SPN (Synthetic preparation); PREP (Preparation)
(aryl, transition metal complexes, octadecyl ether derivs., preparation and film formation and potential use of, in gas sensors)

IT Sensors
(gas, optical, metal complexes with octadecyl ether derivs. of (hydroxyphenyl)porphyrins for)

IT 151866-33-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and UV spectrum of)

IT 151866-31-8P 151866-34-1P 151866-35-2P 151866-37-4P 151894-12-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and film formation and optical behavior of, in presence of gases)

IT 151866-28-3P 151866-29-4P 151866-30-7P 151866-32-9P 151866-36-3P **151894-13-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and film formation with stearic acid and optical behavior of, in presence of gases)

IT 13963-57-0, Aluminum acetylacetonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (hydroxyphenyl)porphyrin octadecyl ethers)

IT 7647-01-0, Hydrochloric acid, reactions 7782-50-5, Chlorine, reactions 10102-44-0, Nitrogen dioxide, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with films of metal complexes with octadecyl ether derivs. of (hydroxyphenyl)porphyrins, UV spectral changes in)

IT 145931-33-5, 5,10,15,20-Tetrakis(hydroxyphenyl)porphyrin octadecyl ether 145931-36-8, 5,10,15,20-Tetrakis(hydroxyphenyl)porphyrin 5,10,15-tris(octadecyl ether)
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with transition metal compds.)

IT 145931-34-6, 5,10,15,20-Tetrakis(hydroxyphenyl)porphyrin

5,10-bis(octadecyl ether)
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with transition metal compds. and refractive index and extinction coefficient of films of, before and after hydrogen chloride exposure)

IT 302-01-2, Hydrazine, uses
RL: USES (Uses)
(resetting reagent, for films of metal complexes with octadecyl ether derivs. of (hydroxyphenyl)porphyrins after exposure to gases)

IT 57-11-4, Stearic acid, uses
RL: USES (Uses)
(stabilizer, for films of metal complexes with octadecyl ether derivs. of (hydroxyphenyl)porphyrins)

IT **151894-13-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and film formation with stearic acid and optical behavior of, in presence of gases)

RN 151894-13-2 HCAPLUS

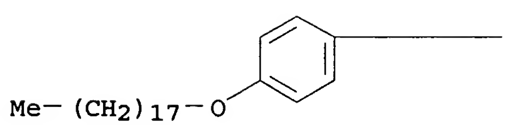
CN Aluminum, bis[μ-[4-[10,15,20-tris[4-(octadecyloxy)phenyl]-21H,23H-porphin-5-yl]phenolato(3-)-N21,N22,N23,N24:O1]]di- (9CI) (CA INDEX NAME)

PAGE 1-A

$Me-(CH_2)_{17}-$

PAGE 1-B

PAGE 2-A



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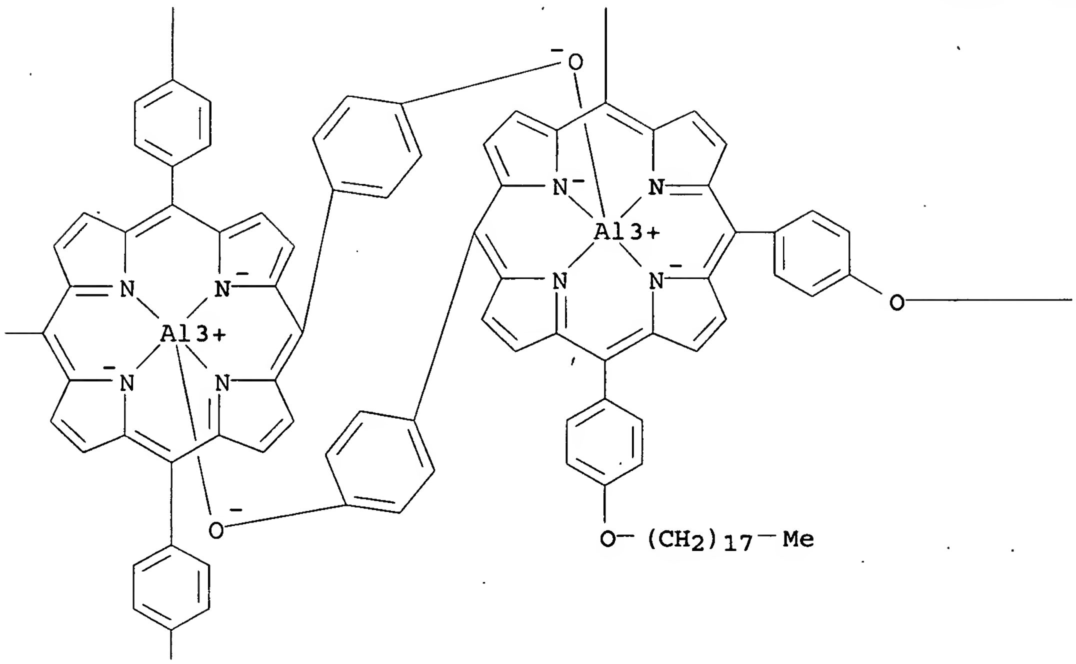


PAGE 2-C

— $(CH_2)_{17}$— Me

PAGE 3-A

Me— $(CH_2)_{17}$—

PAGE 3-B

L47 ANSWER 51 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:664181 HCAPLUS
DOCUMENT NUMBER: 115:264181
TITLE: In situ XANES of an iron porphyrin irreversibly adsorbed on an electrode surface
AUTHOR(S): Kim, Sunghyun; Bae, In Tae; Sandifer, Marnita; Ross, Philip N.; Carr, Roger; Woicik, Joseph; Antonio, Mark R.; Scherson, Daniel A.
CORPORATE SOURCE: Case Cent. Electrochem. Sci., Case West. Reserve Univ., Cleveland, OH, 44106, USA
SOURCE: Journal of the American Chemical Society (**1991**), 113(24), 9063-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In situ Fe K-edge x-ray absorption near edge structure (XANES) was used to examine the axial coordination of (μ-oxo)bis [iron meso-tetrakis(methoxyphenyl)porphyrin] (FeTMPP)2O) irreversibly adsorbed on a high area carbon **substrate** (Black Pearl (BP)) as a function of applied potential. Anal. of the XANES provides conclusive evidence that the coordination around $Fe(3+)$ in the supported, fully oxidized macrocycle is remarkably different from that around $Fe(2+)$ in the corresponding fully reduced macrocycle. In the adsorbed, oxidized state, (FeTMPP)2O retains its μ-oxo character and it undergoes a two-electron reduction to yield predominantly 4-coordinate square-planar FeTMPP without axial ligation.
CC 66-4 (Surface Chemistry and Colloids)
Section cross-reference(s): 72, **73**, 78
ST adsorbed iron porphyrin carbon electrode coordination; x ray spectra adsorbed macrocycle electrochem; oxidized iron porphyrin adsorbed carbon electrode
IT Adsorbed substances
(iron porphyrin complex, on carbon electrode, x-ray absorption near edge structure study of coordination state of)
IT Electric potential
(redox, of iron porphyrin complex adsorbed on carbon)
IT **37191-17-6** 57715-41-0
RL: PRP (Properties)
(adsorbed, on carbon electrode, x-ray absorption near edge structure of coordination state of)
IT 7440-44-0, Carbon, uses and miscellaneous
RL: USES (Uses)
(electrodes, adsorbed iron porphyrin complex on, x-ray absorption near edge structure study of)
IT **37191-17-6**
RL: PRP (Properties)
(adsorbed, on carbon electrode, x-ray absorption near edge structure of coordination state of)
RN 37191-17-6 HCAPLUS
CN Iron, μ-oxobis[5,10,15,20-tetrakis(4-methoxyphenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L47 ANSWER 52 OF 56 HCAPLUS
ACCESSION NUMBER: 1991:530757 HCAPLUS
DOCUMENT NUMBER: 115:130757
TITLE: Photoinitiated vectorial transmembrane electron transfer in bilayers sensitized by a face to face triporphyrin acting as a **molecular** electronic **device.** Amplification due to

ionic coupling

AUTHOR(S): Lamrabte, A.; Janot, J. M.; Bienvenue, E.; Momenteau, M.; Seta, P.
CORPORATE SOURCE: Lab. Physicochim. Syst. Polyphases, CNRS, Montpellier, 34033, Fr.
SOURCE: Photochemistry and Photobiology (**1991**), 54(1), 123-6
CODEN: PHCBAP; ISSN: 0031-8655
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Under light excitation, transmembrane electron transfer is observed when a stacked Zn-Cu-Zn triporphyrin is incorporated in a bilayer between aqueous redox phases. The elec. polarization of the membrane due to the photoinduced transmembrane charge flux drives ion transport. This effect increases the net charge transfer across the system, giving rise to an amplification similar to a field effect transistor. Thus, this system can be considered an organic phototransistor.
CC 8-10 (Radiation Biochemistry)
Section cross-reference(s): 6
ST triporphyrin photosensitization electron transfer blood membrane
IT Electron transport system, biological
(in lipid bilayer membrane, photoinitiation of, by zinc-copper-zinc triporphyrin)
IT Photodynamic action
(of zinc-copper-zinc triporphyrin, on electron transfer in lipid bilayer membranes with visible light)
IT Light, biological effects
(sensitization to, of electron transfer in lipid bilayer membranes by zinc-copper-zinc triporphyrin)
IT Membrane, biological
(bilayer, electron transfer in, photoinitiation of, by zinc-copper-zinc triporphyrin)
IT Transistors
(photo-, organic, zinc-copper-zinc triporphyrin-containing lipid bilayer membranes as)
IT **131687-43-9**
RL: BIOL (Biological study)
(photosensitization by, of electron transfer in lipid bilayer membranes)
IT **131687-43-9**
RL: BIOL (Biological study)
(photosensitization by, of electron transfer in lipid bilayer membranes)
RN 131687-43-9 HCAPLUS
CN Copper, [μ3-[7,22,24,25,26,27,28,29,30,31,32,33,52,67,69,84,86,87,88,89,90,91,92,93,94,95-hexacosahydro-5H,112H-13,16:41,44:58,61:75,78:103,106:120,123-hexaimino-12,40:17,45:57,119:62,124:74,102:79,107-hexa[2]pyrrolyl[5]ylidenedodecabenzo[d,l,q,y,o1,w1,b2,j2,o2,w2,m3,u3][1,3,14,16,27,40,51,53,64,66,77,90]dodecaazacyclohectane-6,23,34,51,68,85,96,113(35H,50H,97H,114H)-octonato(6-)-N126,N130,N132,N148:N137,N141,N143,N147:N150,N154,N156,N160]]bis(zinc)- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L47 ANSWER 53 OF 56 HCAPLUS
ACCESSION NUMBER: 1990:510635 HCAPLUS
DOCUMENT NUMBER: 113:110635
TITLE: Influence of soil substrate and ozone plus acid mist on the pigment content and composition of needles from

young Norway spruce trees

AUTHOR(S): Senser, M.; Kloos, M.; Luetz, C.
CORPORATE SOURCE: Bot. Inst., Univ. Muenchen, Munich, D-8000/19, Germany

SOURCE: Environmental Pollution (Oxford, United Kingdom) (**1990**), 64(3-4), 295-312
CODEN: ENPOEK; ISSN: 0269-7491
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The influence of an ozone + acid mist treatment on photosynthetic pigments has been examined with the needles of the Picea abies clones 11, 14, 16, and 133. At the end of the 14-mo. experiment, which incorporated frost events during a simulated winter period, neither symptoms corresponding to those of spruce type I or IV decline, nor those of ozone damage could be observed However, the 1986 needles of the trees on soil 1, which exhibit an adequate nutrient content, showed zonal chlorosis independently of the ozone + acid mist treatment. Anal. of variance of chlorophyll contents and needle ages showed a clear reduction to nearly 50% in the 1986 needles of clone 11, soil 1, and clone 16, soil 2. In contrast, clones 14 and 16 (soil 1) formed significantly more chlorophylls during the shorter exposure time in the 1987 flush. The detailed anal. of the individual pigment components of clone 14 needles provided no evidence for a destructive influence of the treatment on the chlorophylls, xanthophylls and β-carotene in the two needle generations which had developed during the experiment, in spite of the distinct K deficiency of the 1986 needles of the trees on soil 2 and the common chlorosis of the needles of the trees on soil 1. The observed increase in violaxanthin content upon O3-treatment observed in clone 14 can be considered as an expression of the protective **function** of the xanthophylls against **photooxidative** processes. In conclusion, the observed differences in the chlorophyll and carotenoid contents are better correlated with the individual clone and soil character than with the ozone + acid mist treatment.

CC 4-3 (Toxicology)
ST Picea pigment acid mist ozone soil; spruce pigment acid mist ozone soil
IT Air pollution
 (acid fog and ozone and soil substrate effect on Norway spruce in relation to)
IT Carotenes and Carotenoids, biological studies
 Chlorophylls, biological studies
 RL: BIOL (Biological study)
 (of Norway spruce needles, acid mist and ozone and soil substrate effect on)
IT Soils
 (acid, Norway spruce needle composition and pigment response to acid mist and ozone and)
IT Fog
 (acid, Norway spruce needle composition and pigment response to ozone and soil substrate and)
IT Soils
 (calcareous, Norway spruce needle composition and pigment response to acid mist and ozone and)
IT Leaf
 (needle, composition and pigments of Picea abies, acid mist and ozone and soil substrate effect on)
IT Carotenes and Carotenoids, biological studies
 RL: BIOL (Biological study)
 (oxy, of Norway spruce needles, acid mist and ozone and soil substrate effect on)
IT Spruce
 (P. abies, acid mist and ozone and soil substrate effect on, needle

composition and pigment response to)

IT 10028-15-6, Ozone, biological studies
RL: BIOL (Biological study)
(Norway spruce needle composition and pigments response to acid mist and soil substrate and)

IT 7440-09-7, Potassium, biological studies
RL: BIOL (Biological study)
(acid mist and ozone and soil substrate effect on Norway spruce needle composition and pigment response to)

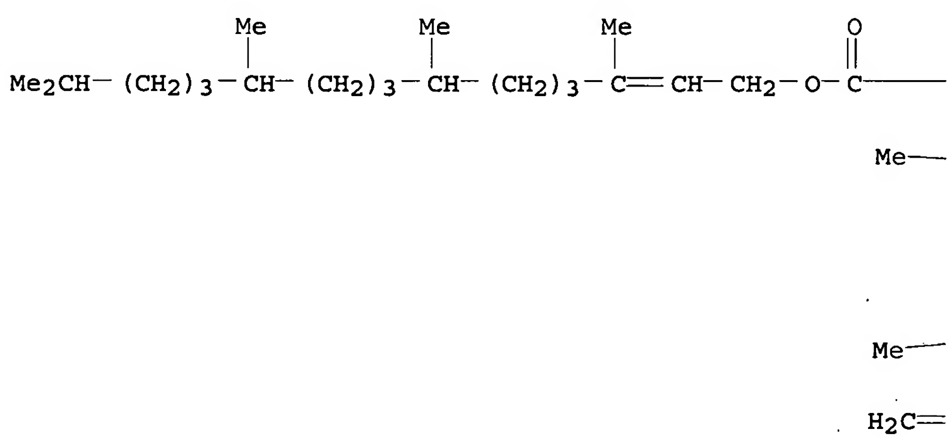
IT 126-29-4, Violaxanthin 127-40-2, Lutein 144-68-3 **479-61-8**, Chlorophyll a **519-62-0**, Chlorophyll b **603-17-8**, Pheophytin a 640-03-9 **3147-18-0**, Pheophytin b 7235-40-7, β-Carotene 14660-91-4, Neoxanthin
RL: BIOL (Biological study)
(of Norway spruce needles, acid mist and ozone and soil **substrate** effect on)

IT **479-61-8**, Chlorophyll a
RL: BIOL (Biological study)
(of Norway spruce needles, acid mist and ozone and soil **substrate** effect on)

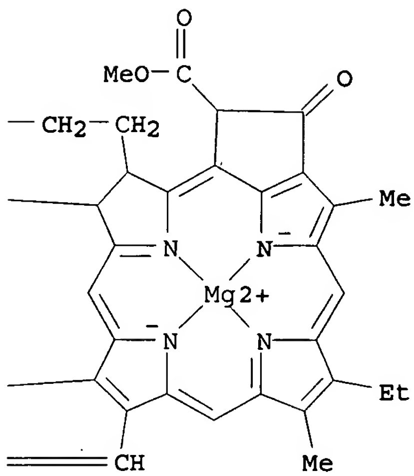
RN 479-61-8 HCAPLUS

CN Magnesium, [(2E,7R,11R)-3,7,11,15-tetramethyl-2-hexadecenyl (3S,4S,21R)-9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-κN23,κN24,κN25,κN2 6]-, (SP-4-2)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L47 ANSWER 54 OF 56 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:14982 HCAPLUS
DOCUMENT NUMBER: 110:14982
TITLE: Electrochemical and surface Raman spectroscopic studies of an iron porphyrin adsorbed on an electrode
AUTHOR(S): Holze, Rudolf
CORPORATE SOURCE: Inst. Phys. Chem., Univ. Bonn, Bonn, D-5300/1, Fed. Rep. Ger.
SOURCE: Electrochimica Acta (**1988**), 33(11), 1619-27
CODEN: ELCAAV; ISSN: 0013-4686
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The adsorption of μ-oxo[meso-tetrakis(methoxyphenyl)porphyrinato]duron by polycryst. Ag, Au and glassy C electrodes and the interaction of the complex with an aqueous electrolyte solution and O dissolved therein were studied by using cyclic voltammetry and surface resonance Raman spectroscopy. Evidence for a redox process is found in the cyclic voltammograms measured with the chelate adsorbed on a glassy C electrode. Spectroscopic results indicate an edge on orientation of the chelate on a Ag electrode, since band shifts of the methoxyphenyl substituent are observed, whereas the remaining spectrum of the adsorbed chelate does not show significant shifts of bands after adsorption on the **substrate.** Upon exposure to an acidic electrolyte solution band shifts indicating association of solution phase components at the porphyrin skeleton are found. In the presence of O2 in the solution phase a new Raman band is observed which can be attributed to an end-on coordinated O2 mol.

CC 72-2 (Electrochemistry)
Section cross-reference(s): 66, **73**, 78
ST adsorption iron oxo methoxyphenylporphyrin electrode; Raman spectra adsorbed iron porphyrin electrode; silver electrode adsorbed iron porphyrin; gold electrode adsorbed iron porphyrin; carbon electrode adsorbed iron porphyrin; oxygen coordination iron porphyrin
IT Adsorbed substances
(iron·oxotetrakis(methoxyphenyl)porphyrindinuclear complex on electrodes, surface Raman spectroscopy in study of)
IT Infrared spectra

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        (of iron oxotetrakis(methoxyphenyl)porphyrindinuclear complex)
IT    Adsorption
        (of iron oxotetrakis(methoxyphenyl)porphyrindinuclear complex by glassy
        carbon or gold or silver electrodes in aqueous solns., surface Raman
        spectroscopy in study of)
IT    Reduction, electrochemical
        (of oxygen on silver electrode with adsorbed iron
        oxotetrakis(methoxyphenyl)porphyrindinuclear complex)
IT    Redox reaction
        (electrochem., of iron oxotetrakis(methoxyphenyl)porphyrindinuclear
        complex adsorbed on electrode in aqueous solns.)
IT    Raman spectra
        (resonance, surface, of iron oxotetrakis(methoxyphenyl)porphyrindinucle
        ar complex adsorbed on electrode)
IT    7440-44-0, Carbon, properties
      RL: PRP (Properties)
        (adsorption by electrode from glassy, of iron
        tetrakis(methoxyphenyl)porphyrinoxodinuclear complex, surface Raman
        spectroscopy in study of)
IT    7440-22-4, Silver, properties   7440-57-5, Gold, properties
      RL: PRP (Properties)
        (adsorption by electrode of, of iron tetrakis(methoxyphenyl)porphyrinox
        oldinuclear complex in aqueous solns., surface Raman spectroscopy in study
        of)
IT    37191-17-6
      RL: PEP (Physical, engineering or chemical process); PROC (Process)
        (adsorption of, by glassy carbon and gold and silver electrodes in aqueous
        solns., surface resonance Raman spectroscopy in study of)
IT    7782-44-7, Oxygen, properties
      RL: PRP (Properties)
        (coordination of, by iron oxotetrakis(methoxyphenyl)porphyrindinuclear
        complex adsorbed on electrode)
IT    59900-45-7P, Gold hydroxide (Au(OH)2)
      RL: PREP (Preparation)
        (formation of, electrochem., on gold, adsorbed iron
        oxotetrakis(methoxyphenyl)porphyrindinuclear complex effect on)
IT    37191-17-6
      RL: PEP (Physical, engineering or chemical process); PROC (Process)
        (adsorption of, by glassy carbon and gold and silver electrodes in aqueous
        solns., surface resonance Raman spectroscopy in study of)
RN    37191-17-6  HCAPLUS
CN    Iron, μ-oxobis[5,10,15,20-tetrakis(4-methoxyphenyl)-21H,23H-
      porphinato(2-)-κN21,κN22,κN23,κN24]di- (9CI)  (CA
      INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L47  ANSWER 55 OF 56  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:        1985:584087  HCAPLUS
DOCUMENT NUMBER:         103:184087
TITLE:                   Surface-enhanced resonance Raman scattering of
                         trivalent metal tetraphenylporphine complexes in a
                         layered structure of a calcium fluoride-roughened
                         substrate/sample/silver
AUTHOR(S):               Takenaka, A.; Takeuchi, S.; Kobayashi, Y.; Itoh, K.
CORPORATE SOURCE:        Sch. Sci. Eng., Waseda Univ., Tokyo, 160, Japan
SOURCE:                  Surface Science (1985), 158(1-3), 359-69
                         CODEN: SUSCAS; ISSN: 0039-6028
DOCUMENT TYPE:           Journal
LANGUAGE:                English
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AB Surface-enhanced resonance Raman scattering spectra were measured for trivalent metal tetraphenylporphine (TPP) complexes, such as Fe(III)TPPCl, Mn(III)TPPCl, and Cr(III)TPPCl, in a layered structure having a CaF2-roughened **substrate**/sample/Ag configuration. Each surface spectrum is appreciably different from the resonance Raman scattering (RRS) spectrum of the corresponding metalloporphine but similar to the RRS spectrum of corresponding μ-oxo dimer ([Fe(III)TPP]2O or [Mn(III)TPP]2) or a monohydroxy complex Cr(III)TPPOH. This result indicates that, when the above-mentioned metalloporphines interact with Ag vapor during its deposition process, the complexes are converted to the μ-oxo dimers and the monohydroxy complex, resp.

CC 66-3 (Surface Chemistry and Colloids)
Section cross-reference(s): **73**

ST metalloporphine Raman adsorbed layered structure; Raman enhanced adsorbed metalloporphine; calcium fluoride roughened **substrate** Raman; silver adsorbate Raman metalloporphine

IT Porphyrins
RL: PRP (Properties)
(metal complexes, adsorbed on silver in layered structure with calcium fluoride-roughened **substrate**, surface enhanced Raman scattering by)

IT Adsorbed substances
(metalloporphyrins, on silver in layered structure with calcium fluoride-roughened **substrate**, surface enhanced Raman scattering by)

IT Raman spectra
(surface-enhanced, of metalloporphyrins adsorbed on silver in layered structure with calcium fluoride-roughened **substrate**)

IT 7440-22-4, properties
RL: PRP (Properties)
(adsorbed metalloporphines on, in layered structure with calcium fluoride-roughened **substrate**, surface enhanced Raman scattering from)

IT **12582-61-5** **12650-83-8** 16456-81-8 28110-70-5
32195-55-4 33519-59-4
RL: PRP (Properties)
(adsorbed, on silver in layered structure with calcium fluoride-roughened **substrate**, surface enhanced Raman scattering by)

IT 7789-75-5, properties
RL: PRP (Properties)
(surface enhanced Raman scattering from metalloporphines adsorbed on silver in layered structure with **substrate** of roughened)

IT **12582-61-5**
RL: PRP (Properties)
(adsorbed, on silver in layered structure with calcium fluoride-roughened **substrate**, surface enhanced Raman scattering by)

RN 12582-61-5 HCAPLUS

CN Iron, μ-oxobis[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L47 ANSWER 56 OF 56 HCAPLUS

ACCESSION NUMBER: 1980:155269 HCAPLUS
DOCUMENT NUMBER: 92:155269
TITLE: Electronic structure of a porphyrin solid film and energy transfer at the interface with a metal substrate

AUTHOR(S): Tanimura, K.; Kawai, T.; Sakata, T.
CORPORATE SOURCE: Inst. Mol. Sci., Okazaki, 444, Japan
SOURCE: Journal of Physical Chemistry (**1980**), 84(7), 751-6
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The electronic structure and the interaction with a metal substrate of amorphous solid films of free base tetraphenylporphine (H2TPP) and its Zn derivative (ZnTPP) were studied. The visible absorption spectra resemble those of solns., although the Soret band is greatly weakened and broadened in the film. The lifetime of the S1 state in an amorphous H2TPP film is less than 2 ns, and is much shorter than that of solns. This quenching is attributed to enhancement of the nonradiative decay rate in the solid phase. The typical effect of the metal substrate on the film is a strong quenching both of sensitized chlorin emission in ZnTPP and of fluorescence in H2TPP. Foerster type energy transfer to the metal substrate explains most of the quenching, but an addnl. long-range effect in the H2TPP film is attributed to exciton diffusion within the film. The metal-dye system is discussed in terms of a **device** for solar-energy conversion.

CC 73-3 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other **Optical** Properties)

ST visible spectra zinc tetraphenylporphine; porphine phenyl zinc luminescence

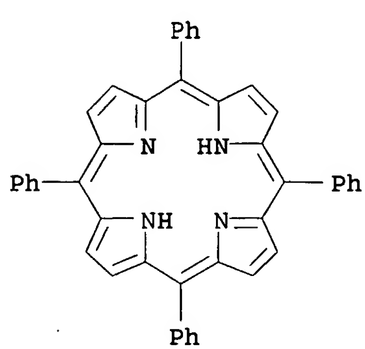
IT Electron configuration
Fluorescence
Fluorescence quenching
Ultraviolet and visible spectra
(of tetraphenylporphine and its zinc derivative at metal substrate interfaces)

IT **917-23-7** **14074-80-7**
RL: PRP (Properties)
(electronic structure and spectral properties of, in solid films and at metal **substrate** interfaces)

IT **917-23-7**
RL: PRP (Properties)
(electronic structure and spectral properties of, in solid films and at metal **substrate** interfaces)

RN 917-23-7 HCAPLUS

CN 21H,23H-Porphine, 5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



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